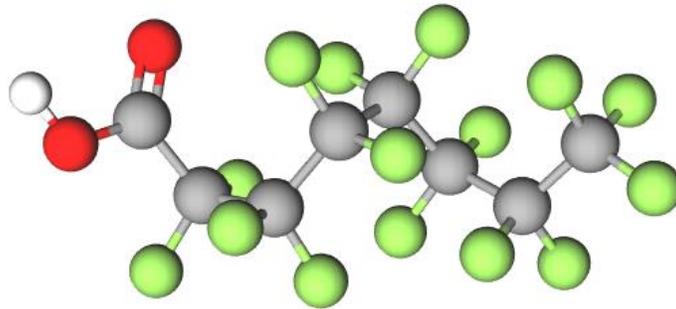


June 2020

REVIEW OF MODELS FOR EVALUATING PER- AND POLYFLUOROALKYL SUBSTANCES IN LAND APPLIED RESIDUALS AND BIOSOLIDS

An Assessment of Fate and Transport Models for
Groundwater Leaching, Surface Water Runoff, and
Plant Uptake



REVIEW OF MODELS FOR EVALUATING PER- AND POLYFLUOROALKYL SUBSTANCES IN LAND APPLIED RESIDUALS AND BIOSOLIDS (V1.1)

REVIEW OF MODELS FOR EVALUATING PER- AND POLYFLUOROALKYL SUBSTANCES IN RESIDUAL AND BIOSOLIDS

An Assessment of Fate and Transport Models for Groundwater Leaching,
Surface Water Runoff, and Plant Uptake

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June 2020

V1.1

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Appendix A Model Screening

Appendix B Summary of Literature-Based Soil to Plants Transfer Factors for Selected PFAS

ACRONYMS AND ABBREVIATIONS

CEAM	Centre for Exposure Assessment Modeling
CN	curve number
CSA	Canadian Standard Association
FTOH	fluorotelemer alcohol
g/L	gram per liter
GUI	graphical user interface
ITRC	Interstate Technology and Regulatory Council
NCASI	National Council for Air and Stream Improvement, Inc.
PFAA	perfluoroalkyl acid
PFAS	per- and polyfluoroalkyl substances
PFCA	perfluoroalkyl carboxylate
PFOA	perfluorooctanoic acid
PFOS	perfluorooctane sulfonic acid
PFOSA	perfluoroalkyl sulfonamide
PFSA	perfluoroalkyl sulfonates
PMRA	Pest Management Regulatory Agency (Canada)
PWC	Pesticide in Water Calculator
RCF	root concentration factor
SCF	shoot-soil concentration factor
SSM	Source Screening Module
TF	transfer factor
USEPA	United States Environmental Protection Agency
USGS	U.S. Geological Survey
VVWM	Variable Volume Water Model

EXECUTIVE SUMMARY

Per- and polyfluoroalkyl substances (PFAS) are a complicated group of more than 3,000 man-made chemicals (ITRC 2017). In the past decade, awareness of the pervasiveness and unique characteristics of PFAS has grown rapidly into the realization that PFAS are ubiquitous in manufactured products, industrial processes, and (as a result) the environment. That realization has prompted an increase in our scientific understanding of PFAS characteristics, fate and transport processes, as well as efforts to mitigate the potential impacts of PFAS.

Our growing understanding includes determining if PFAS are present in wastewater treatment residuals from manufacturing sources (e.g., pulp and paper wastewater residuals) and biosolids from municipal wastewater utilities (collectively referred to as residuals herein) and assessing the potential for PFAS in soils amended with wastewater residuals to migrate into other environmental media such as groundwater, plants, or surface water. In response to the potential migration to other media, regulatory agencies have begun to evaluate the fate, transport, and effects of PFAS in land-applied residuals and, in some cases, develop guidelines to mitigate potential effects. Fate and transport models are critical to evaluating and establishing appropriate guidelines to developing screening levels. However, because of the unique properties of PFAS, it is unclear if current models are capable of adequately modeling PFAS fate and transport.

This report reviews available fate and transport models for the three primary migration pathways for PFAS in land-applied residuals: leaching to groundwater, surface water runoff, and plant uptake. Numerous models are available, but only a few are likely to be applicable to PFAS and able to account for their unique and diverse physicochemical characteristics. This review is intended to assist policy makers, regulators, and industry in their consideration of fate and transport models to apply when evaluating potential effects of PFAS in land-applied residuals and establishing appropriate screening values for PFAS in such residuals.

Models were identified by reviewing government compilations and conducting online searches for models used in North America. Models were then screened based on criteria of applicability, peer review status, availability of updates and support, and accessibility of the model (Appendix A). Retained models were further evaluated for their ability to accurately simulate PFAS transport and account for processes and parameters that are likely to have substantial influence on the fate and transport of PFAS in land-applied residuals (Tables 2 through 4). The mechanisms and processes affecting PFAS transport through the three migration pathways listed below were examined as part of the screening process.

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Leaching		
Advection*	Sorption*	Volatilization
Diffusion/dispersion	Electrostatic bonding	Dual domain
Degradation	Air-water interface partitioning*	Surface tension
PFAS Transformation*		
Surface Water Runoff		
Sorption*	Air-water interface partitioning*	Electrostatic adsorption
PFAS Transformation*		
Plant Uptake		
Sorption/Desorption	Soil-to-plant transfer factors*	Tissue-to-tissue transfer factors
Transpiration	Translocation	Metabolism and growth dilution
PFAS Transformation*		

* = indicates a parameter critical to PFAS modeling for the respective pathways

The outcomes of the reviews are summarized below for each of the migration pathways.

Leaching Model Review

Thirty-one models were reviewed for the leaching pathway, of which three were identified as having the potential to model PFAS leaching, listed below in alpha-numeric order.

- Hydrogeochem (4.0/5.0)
- Hydrus (1D, 2D, and 3D)
- SVENVIRO™.

These three models are robust, well maintained, well documented and reviewed. Further, these models are the most likely to be updated to adopt additional key PFAS modeling parameters, like air-water interface partitioning (K_{ia}). None of the models reviewed can model all the key parameters that affect PFAS leaching from land-applied residuals (e.g., K_{ia}). Like all other models reviewed in this report, these three leaching models do not have the ability to model K_{ia} . Because K_{ia} , when present, is assumed to act as a mechanism that limits the mass of PFAS available to leach from land-applied residuals, the inability of these models to account for such partitioning is likely to result in the models overestimating, rather than underestimating, the concentration of PFAS in leachate that may reach groundwater. Such overestimates of PFAS concentrations in leachate may be acceptable depending on the purpose of the application of the models (e.g., developing conservative estimates of PFAS concentrations in leachate). Additional research will likely be necessary to understand how accurately the existing models are able to simulate PFAS leaching under a variety of conditions, whether additional model development may be necessary to improve predictive ability, and the degree of improvement in predictions such additional development is likely to garner.

The other vadose zone leaching models identified may also be suitable for PFAS modeling but were considered less applicable as summarized in Section 2.2 and Table 2. These models were too complex for the typical user, lacked key modeling capabilities, exhibited documented limitations, and/or were not adequately maintained or supported. However, they could be used if the limitations are appropriately accounted for.

Surface Water Runoff Model Review

Thirty models were reviewed for the surface runoff pathway, of which one model was identified as having the greatest potential to model PFAS runoff to surface water. Pesticide in Water Calculator (PWC) was identified as the most applicable to modeling PFAS at a field scale, where residuals are applied to a plot of land and PFAS concentrations in runoff need to be modeled. PWC was selected for its ability to model runoff as part of a water balance and its ability to characterize the interaction of soil with water (not just sheet flow, as do other models), for its range of landcover scenarios, for the ability to enter site-specific weather data, and that applicable chemical-specific inputs that can be incorporated. In addition, transport-specific functions in the model handle complex, nonlinear, and nonequilibrium situations that may be exhibited by PFAS.

One of the limitations of PWC, and virtually all other models, is the inability to account for K_{ia} and the surface tension effects. While it is unclear exactly how K_{ia} and the surface tension effects of PFAS will affect surface water runoff from land-applied residuals, it is expected to be relatively minor because PFAS porewater concentrations in runoff from land-applied residuals are expected to be in the milligram per liter range or less, and the surface water runoff will effectively saturate surrounding soils, reducing air space, and thus reducing the effects of K_{ia} on runoff transport.

Plant Uptake Model Review

Twelve plant uptake models were identified and reviewed, of which only two were retained for further evaluation. While these two models appear to have the capability to model the uptake of PFAS by plants, they require plant-specific and PFAS-specific inputs that are not currently available for most plant species and PFAS. However, soil-to-plant transfer factors (TFs) are available for a range of plant species and several individual PFAS. Until the required information is available for the two retained plant uptake models, soil-to-plant TFs from the literature can be used to estimate accumulation of PFAS in plants.

Because a publicly available database of TFs is not currently available, a compilation of literature-based soil-to-plant and soil solution-to-plant TFs for PFAS is presented in this report (Table B-1) and provides TFs for several PFAS in a variety of crop species. Two general, but not universally consistent, trends in soil-to-plant TFs are apparent. The first is that TFs tend to decrease with increasing PFAS carbon chain length. This trend in TFs of perfluoroalkyl acids (PFAAs) is consistent with findings of other studies (e.g., Blaine et al. 2013, 2014a, 2014b; Krippner et al. 2015). The second is that TFs for perfluoroalkyl sulfonates (PFSA) tend to be somewhat lower than TFs for perfluoroalkyl carboxylates (PFCA) in the same plant species and tissue type.

The compilation (Table B-1) can also be used to identify additional data needs and research priorities to enhance the understanding of bioaccumulation of PFAS under various field and test conditions. Examples of such additional evaluations include developing TFs based on regression analysis rather than a simple ratio of concentrations in paired plant tissue and soil samples. The compiled TFs from the literature could also be further explored to look for relationships between TFs and soil characteristics, plant species or tissue types, and PFAS homologues.

Summary

The review of available models found that no single currently available software package can evaluate migration of PFAS through all three pathways, and no models can evaluate all key PFAS parameters for the respective pathways. Therefore, a combination of models will be necessary to evaluate the three migration pathways. When running a combination of models for the three migration pathways, practitioners will need to consider mass conservation. Further, practitioners will need to account for the key PFAS parameters, precursor transformation, and other relevant modeling factors (e.g., residual application rate) and apply professional judgement based on site-specific circumstances.

This review identified some additional research and development needs: 1) accounting for air-water interface partitioning of PFAS in runoff and especially leaching models; 2) accounting for surfactant-induced flow in leaching models; 3) developing more rigorous soil-to-plant TFs using regression analysis; and 4) running currently available models at actual land-applied residual sites to evaluate whether the predictive ability of current models meets the needs of stakeholders associated with such sites.

1 INTRODUCTION

Per- and polyfluoroalkyl substances (PFAS) are a complicated group of more than 3,000 man-made chemicals (ITRC 2017). In the past decade, awareness of the pervasiveness and unique characteristics of PFAS has grown rapidly, and scientists are realizing that PFAS are ubiquitous in manufactured products, industrial processes, and (as a result) the environment. Coupled with that realization has been an increase in our scientific understanding of PFAS characteristics, fate and transport, as well as regulations to mitigate the potential effects of PFAS. That growing understanding includes determining if PFAS are present in wastewater treatment residuals from manufacturing sources (e.g., pulp and paper wastewater residuals) and biosolids from municipal wastewater utilities (collectively referred to as residuals herein) and assessing the potential for PFAS in soils amended with wastewater residuals to migrate into other environmental media such as groundwater, surface water, or plants. The leaching to groundwater pathway may represent the more critical transport pathway given the known migration of PFAS to groundwater and the direct potable use of groundwater.

In response to the potential migration to other media, regulatory agencies and the industry have begun to evaluate the fate, transport, and effects of PFAS in land-applied residuals and, in some cases, developing guidelines to mitigate potential effects. Fate and transport models are critical to such evaluations. However, because of the unique properties of PFAS, it is unclear if current models are capable of adequately modeling PFAS fate and transport, particularly to groundwater.

This report presents a review of available models for three key fate and transport pathways for chemicals in soils and the applicability of these models to PFAS. The three pathways are leaching to groundwater, runoff to surface water, and uptake by plants. Many models are available, but only a few are likely to be applicable to PFAS and able to account for their unique and diverse physicochemical characteristics. This review is intended to assist policy makers, regulators, and industry in their consideration of fate and transport models to apply when evaluating the potential effects of PFAS in land-applied residuals and establishing screening values for PFAS in such residuals. More detailed information regarding PFAS background, regulations, chemistry, naming conventions, and characteristics, is available in ITRC 2017 and Bell et al. 2019.

The remainder of this Introduction presents a brief overview of PFAS and migration pathways from land-applied residuals (Section 1.1), key physicochemical characteristics of PFAS that affect their fate and transport in the environment (Section 1.2), an overview of the relative importance of key model input parameters (Section 1.2.3), and a description of the process used to identify and screen the models included in this review (Section 1.3). The Introduction is followed by the review of leaching models (Section 2), the review of surface water runoff models (Section 3), the review of plant uptake models (Section 4), and conclusions and recommendations (Section 5). References are presented in Section 6 followed by tables and appendices.

1.1 Overview of PFAS in Residuals

PFAS are a complex, large group of synthetic chemicals composed of highly fluorinated alkyl chemicals with diverse properties (NEBRA 2018). PFAS compounds are key in the manufacture of many industrial products, present in firefighting foams, and present in many household items (e.g., carpets and pizza boxes; NEBRA 2018).

The ubiquity of PFAS use in firefighting, industrial processes, and commercial products leads to the creation of physical areas that have the potential to be a source of PFAS to the environment (e.g., airfields, industrial and manufacturing facilities, landfills, resource recovery plants, and soils amended with wastewater treatment residuals; NEBRA 2018). PFAS in wastewater residuals are of particular interest because of the widespread practice of land application of such residuals.

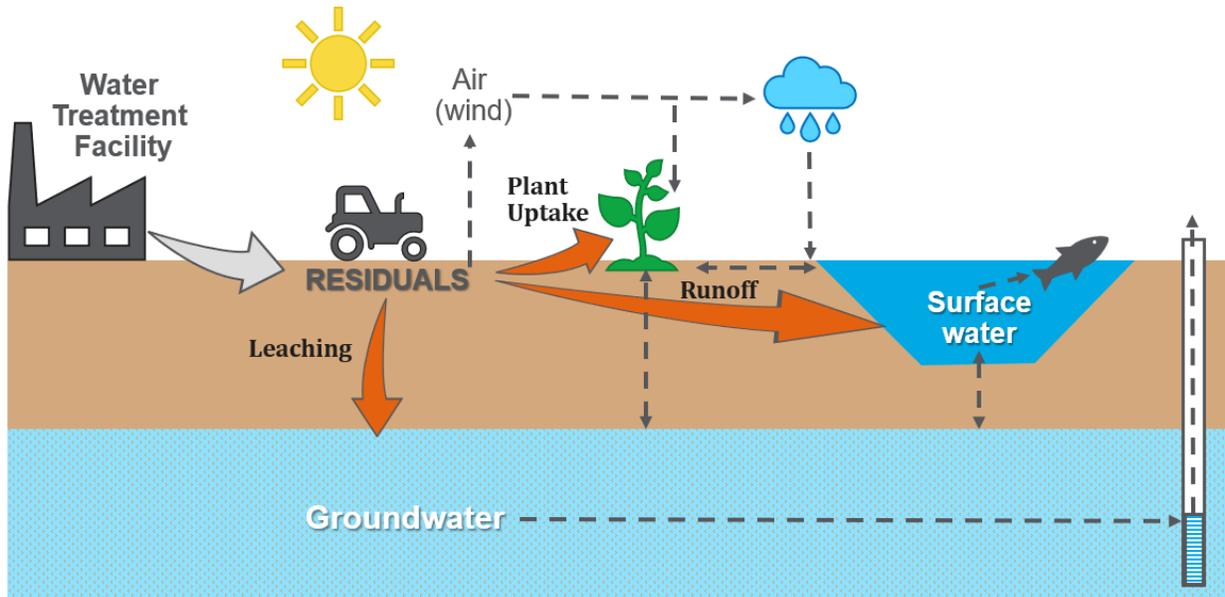
The benefits from land application of residuals for both soil and vegetation are numerous and well recognized. The chemical and physical properties of these residuals make them ideal for land application. They can be a source of slow-release macronutrients (e.g., nitrogen and phosphorus) and micronutrients (e.g., calcium, iron, magnesium, and zinc), which promote plant growth at the application site, leading to increased site productivity. They can also be used to amend soil properties by decreasing bulk density and increasing the water-holding capacity, plant available water, hydraulic conductivity, organic carbon content, and cation exchange capacity. The increase in soil carbon content and site productivity can also have net greenhouse gas benefits.

Given the characteristics of PFAS and nature of residuals, PFAS bound to residuals may be susceptible to desorption and mobilization. Some PFAS found in residuals can transform to more mobile perfluoroalkyl acid (PFAA) forms (NEBRA 2018).

Three processes by which PFAS in residuals may be mobilized and migrate out of land-applied residuals are considered in this review. These include: leaching to groundwater, surface water runoff, and uptake by plants (orange arrows in Exhibit 1). For convenience, this report refers to those three processes as migration pathways, even though uptake by plants is not strictly a migration pathway in the classic interpretation of that term. While other migration pathways are possible (e.g., suspension of particulate bound PFAS in air by wind; dashed grey arrows in Exhibit 1), these three are the primary, initial migration pathways associated with land-applied residuals and have the greatest potential to affect human receptors through impacts to drinking water supplies or crops used for human consumption. Past studies have shown that, due to their ubiquitous nature, perfluorooctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS) are commonly present in land-applied residuals at detectable levels (NEBRA 2018). Residuals generated from areas with direct industrial contributions (i.e., facilities that use PFAS in their operations or manufacturing) generally exhibit the highest concentrations, but PFAS can be found in most residuals, regardless of water source contributors (Koch 2015). When these residuals are applied to soils as part of residuals management practices, PFAS can be introduced to the environment (Exhibit 1).

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Exhibit 1. Primary Migration Pathways for PFAS in Land-Applied Residuals



Solid orange arrows in Exhibit 1 are the primary transport pathways evaluated in this review. The dashed gray arrows represent secondary potential transport pathways.

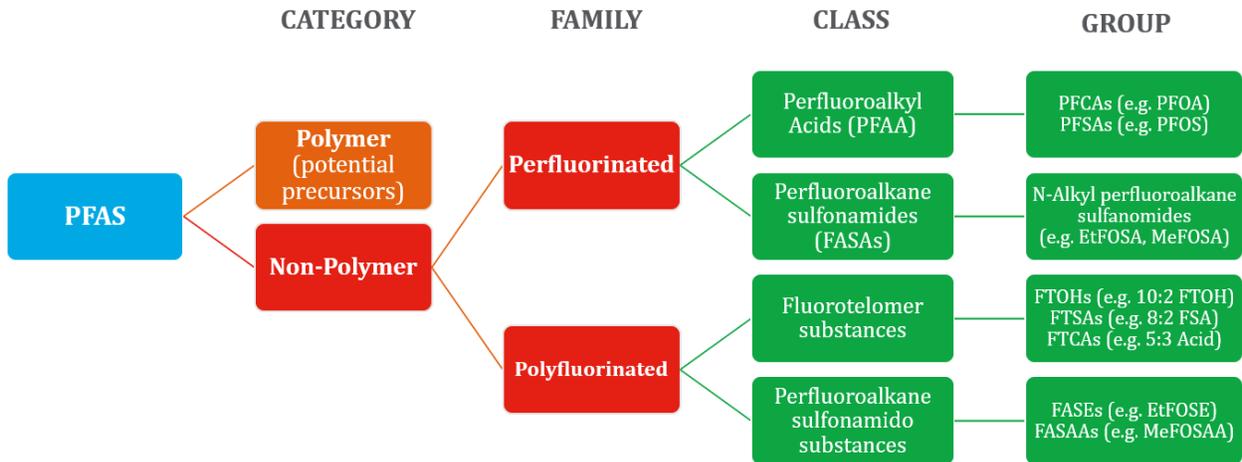
PFAS concentrations show a proportional correlation to the residuals loading rate, particularly for longer-chain perfluoroalkyl carboxylic acids (PFCA; Washington et al. 2009). Short-chain PFAS concentrations in groundwater and surface water also tend to show a proportional correlation with residual loading rates (NEBRA 2018). These concentrations may change over time, with depth, pH, and as a function of precursor degradation as mobility varies with chemical structure (Rankin et al. 2016; Sepulvado et al. 2011). PFAS do move through vadose-zone soils to groundwater, showing strong positive correlations with residual loading rates (both in groundwater and surface water; NEBRA 2018; Sepulvado et al. 2011).

1.2 PFAS Fate and Transport

PFAS is a group of more than 3,000 man-made constituents (ITRC 2017) and is composed of two primary categories (polymer and non-polymer; ITRC 2017). The polymer PFAS are not bioavailable due to their large molecular size (NEBRA 2018). The non-polymer family is further divided into two families: (1) perfluoroalkyl and (2) polyfluoroalkyl non-polymer substances. The perfluoroalkyl substances are fully fluorinated, while the polyfluoroalkyl substances contain a perfluoroalkyl group as well as an alkyl group that is not saturated with fluorines. Exhibit 2 summarizes the general PFAS family, class, and group organization. PFAS are also often divided into short- and long-chain compounds based on the length of their perfluoroalkyl group. PFAS molecules contain a hydrophobic and lipophobic perfluoroalkyl chain, have a high affinity for proteins, have no natural counterparts, and can be readily transported by water (NEBRA 2018). This results in a family of compounds that are mobile and present in nearly all environments including groundwater. The functional groups, chain lengths (generally categorized as short and long chain), and individual characteristics of a PFAS constituent affect its fate and transport. A high-level summary of PFAS nomenclature is presented in Exhibit 2 below.

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Exhibit 2. PFAS Families and Groups



1.2.1 Transport

The principal PFAS-specific factors that affect PFAS partitioning within soil, groundwater, surface water, and sediment are the charge(s) on the PFAS molecule, the length of the perfluoroalkyl chain, and (for PFAA precursors) the structure of the non-fluorinated part of the molecule. Hydrophobic adsorption is the main known retardation mechanism for PFAS with six or more perfluorinated carbons (C), and empirical organic carbon partitioning factors are available for many PFCAs and PFSAAs (Guelfo and Higgins 2013, Higgins and Luthy 2006, Barzen-Hanson et al. 2017, Anderson et al. 2019).

PFAS are relatively soluble, with PFAS aqueous solubility of the C4 to C8 perfluoroalkyl carboxylates and sulfonates ranging from 0.5 gram per liter (g/L) to completely miscible (as summarized in Pancras et al. 2016). Perfluoroalkyl carboxylates are more soluble than perfluoroalkyl sulfonates that contain the same perfluoroalkyl chain length. Groundwater PFAS concentrations have not been reported above the double-digit milligrams per liter range at PFAS firefighting foam-impacted sites (Schultz et al. 2004, Anderson et al. 2016); therefore, modeling of PFAS transport is unlikely to be influenced by solubility limits.

A recently conducted meta-analysis of all source zone PFAS data collected at 324 U.S. Air Force sites provides perhaps the best comprehensive insights into the soil factors governing anionic PFAS transport in soil and groundwater. For a suite of 18 neutral and anionic PFASs, total organic carbon exhibited the most significant positive correlation with observed soil to groundwater ratios for all PFAS (Anderson et al. 2019). The percentage of clay was inversely related to soil-to-groundwater ratios, a phenomenon that the authors attributed to more air-water interfacial partitioning of PFAS occurring during unsaturated flow in soils with less clay. Soil-water partitioning coefficients for PFAS are summarized by ITRC (2018).

In unsaturated materials, significant air-water interfacial partitioning can occur for PFAS (Brusseu 2018, Lyu et al. 2018), resulting in increased storage and retardation of PFAS. Air-water interfacial partitioning occurs when constituents preferentially align themselves along the interface between porewater and air. Schaefer et al. determined that a Freundlich-based model best described PFOS and PFOA uptake at the air-water interface, and that this uptake phenomenon increases with decreasing PFAS concentrations (2019). As a result, PFAS presence in unsaturated residuals may demonstrate less potential for leaching

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relative to saturated residuals. Additionally, as PFAS migrate downwards through the vadose zone, air-water interfacial partitioning will slow PFAS migration.

While some studies have indicated that PFAS exhibit some irreversible adsorption (Milinovic et al. 2015, Miao et al. 2017), the Air Force source zone analysis did not confirm this hysteresis effect (Anderson et al. 2019). Further, a recent laboratory study by Brusseau et al. noted that PFOS sorption and desorption are significantly rate limited, and the influence of non-linear, hysteretic, and irreversible sorption/desorption on the transport of PFAS in soil was minimal (Brusseau et al. 2019b). This means it takes longer for PFAS to desorb and flush from soils.

Electrostatic adsorption mechanisms are potentially important for PFAS with positively charged features, as they are more likely to strongly sorb to the negatively charged soils frequently encountered in the subsurface (Mejia Avendano et al. 2017, Barzen-Hanson et al. 2017). The overall soil-water partitioning coefficient (K_d) will reflect the electrostatic adsorption mechanisms for these compounds. Because K_d is site-specific, and few laboratories can measure cationic PFAS, their significance to residuals leaching may be difficult to assess on a wide, representative scale. However, cationic precursors and the slow bio-transformation processes may constitute a long-term relatively immobile source for PFAS in biosolids.

Surfactant-induced flow occurs when the surfactant reduces surface tension of the water-air-soil interface, thereby inducing groundwater flow. Surfactant-induced porewater flow is concentration-dependent and is expected to influence groundwater flow and ultimately transport in the vadose zone when concentrations are in the milligram per liter range in porewater (Guo et al. 2020).

Most PFAS commonly included in laboratory analytical programs are present in an anionic form at environmentally relevant pH because they have very low pK_a values. As a result, PFCAs, PFSAAs, and many precursors are not subject to losses through volatilization. Some PFAS, such as the fluorotelomer alcohols, are volatile. These compounds may be subject to loss in ambient air and soil vapor; however, they may still preferentially sorb to soils. It is unclear how relevant volatile PFAS may be to biosolids and other residuals, as data on these compounds in biosolids have not been reported.

Bioaccumulation of some PFAS has been described for a number of plant species, including differential uptake within different compartments (e.g., roots vs. leaves). Section 4 presents a review of plant uptake models and a summary of soil-to-plant transfer factors.

1.2.2 Fate

No degradation of the perfluoroalkyl sulfonates (PFSAAs) and PFCAs is expected to occur, either in residuals or after they migrate into runoff, groundwater, or plants. Huang and Jaffe have recently reported PFOA and PFOS degradation in the presence of an autotrophic bacteria; however, the results have not been replicated outside of a laboratory environment, and PFCAs and PFSAAs are not considered naturally biodegradable (Huang and Jaffe 2019). In the presence of aerobic bacteria, perfluoroalkyl sulfonamide (PFOSA) precursors have been shown to slowly biotransform to PFSAAs (Mejia Avendano et al. 2016; Rhoads et al. 2008), and fluorotelomer precursors have been shown to degrade somewhat more rapidly to PFCAs (Wang et al. 2005; Lee et al. 2010; Wang et al. 2011; Wang et al. 2009; Liu et al. 2010; Dasu et al. 2012; Harding-Marjanovic et al. 2015). In each of these studies, half-lives of the initial fluorotelomer precursor were on the order of 10 to 20 days, with the production of a number of intermediate polyfluorinated compounds observed. The yield of PFCA terminal products was less than 10 percent over

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the duration of the experiment (typically two to three half-lives), suggesting that, even under optimal conditions, biotransformation of PFAA precursors to terminal PFAAs is relatively slow. The few studies investigating biotransformation of PFAA precursors under anaerobic conditions suggest that half-lives of PFAA precursors, even with fluorotelomer structures, are at least months long; while some transformation to intermediate structures occurs, often via different pathways than under aerobic conditions, production of terminal PFAA products has not been observed over half-year or longer durations (Zhang et al. 2013; Zhang et al. 2016; Yi et al. 2018).

When accounting for potential precursor transformation to PFAAs in residuals leaching and uptake models, it is too conservative to assume that all precursors will transform to PFAAs. If precursors can be measured, then transformation may be estimated according to redox conditions. A nominal value of 5 to 10 percent conversion of precursors per year to corresponding PFCAs or PFSAs may be a reasonable rate under aerobic conditions. Stability of precursors in initial or intermediate forms may be assumed under oxygen-depleted redox conditions.

1.2.3 Key Fate and Transport Parameters for Modeling PFAS

Table 1 summarizes the key fate and transport parameters specific to modeling PFAS for the three migration pathways evaluated herein. Exhibit 3 below summarizes the key modeling parameters and their relative importance when modeling the three migration pathways. Additional discussion of each parameter and its importance is provided in Section 1.2 and Table 1.

Exhibit 3. Relative Importance of Parameters in Modeling PFAS Fate and Transport

Effect of Input Parameter on Model Prediction	Leaching to Groundwater	Surface Water Runoff	Plant Uptake
Hydrophobic Adsorption and Desorption	High	High	High
Soil-to-plant Transfer Factor	Low	None	High
PFAA Generation from Precursors	Moderate/High*	Moderate/High*	Moderate/High*
Air-Water Interface Partitioning	Moderate to High	Moderate to Low	Moderate
Electrostatic Adsorption	Moderate	Moderate to Low	Moderate to Low
Solubility	Low#	Low#	Low#
Surface tension	Moderate to Low	Low	Low
Volatilization	Low	Low	Low
Fluorophilic Interactions	Low	Low	Low
Decay	None	None	None

Notes:

* = may act as an ongoing long-term source of PFAAs

= PFAS solubility is high relative to the concentrations observed in the environment (i.e., all PFAS in residuals will be in the dissolved phase or adsorbed). Thus, solubility limits do not generally affect the modeling of PFAS transport in the environment.

The input parameters described above are specific to the models used to predict the concentrations of PFAS in water leaching from soils that have been amended with residuals containing PFAS, in water running off of such soils and taken up by plants from soils that have been amended with residuals containing PFAS. Application of these models to predict concentrations in groundwater, surface water or

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plants will require additional information or modeling beyond that included in this review. Most obviously, the concentrations of PFAS in amended soil are needed. That concentration may be measured, or it can be predicted using a model. Such models are likely to require, at a minimum, the concentration of PFAS in the residuals, the application rate, the frequency of application, the method of application and mixing depth. PFAS concentrations in residuals will vary significantly based on source material – typical municipal residuals have been reported to contain tens to several hundred micrograms per kilogram ($\mu\text{g}/\text{kg}$) of individual PFAS (Sepulvado et al. 2011, Venkatesan et al. 2013), while concentrations of up to 3,000 $\mu\text{g}/\text{kg}$ PFOS have been observed in manufacturing-impacted biosolids (3M 2001). In the organic fraction of municipal solid waste compost, PFAA concentrations ranged from 28.7 to 75.9 $\mu\text{g}/\text{kg}$ for composts that included food packaging and from 2.38 to 7.60 $\mu\text{g}/\text{kg}$ for composts that did not include food packaging (Choi et al. 2019). PFAS concentrations in soil have been observed to scale with residuals loading rates and decrease with depth (Sepulvado et al. 2011). For a municipal biosolid without any suspected PFAS point source impacts, 0.0151 $\mu\text{g}/\text{kg}$ PFOA was measured in soil per Megagram/hectare of biosolid applied (Sepulvado et al. 2011).

PFAS concentrations in land applied residuals can increase if repeated land applications occur but will be reduced, when the residuals are tilled or mixed with soils. Once the concentration of PFAS in amended soil is known, if the goal is to estimate concentrations in plants, the species of plants grown on amended soil will need to be considered. If estimating concentrations in groundwater from leaching is the goal, various soil properties, size of amended soil area, climate, presence of irrigation, and depth to groundwater will be needed. If estimating concentration in surface water receiving runoff is the goal, in addition to several of the factors noted above for leaching, distance to the nearest surface water, topography, vegetative cover, and various surface water characteristics will be needed.

Finally, if all three migration pathways exist, mass balance should be considered to ensure that the mass of PFAS estimated to be leaving amended soil does not exceed the mass that was present in applied residuals. The approach will vary depending on the circumstances and uncertainty around the practices and pathways. If the estimated losses from all pathways combined is a small fraction of the mass of PFAS in applied residuals, then the models for each pathway can likely be run independently without consideration of losses from the other pathways. However, if losses from one or more of the pathways approach the mass of PFAS in applied residuals, the reduction in PFAS mass available for migration via the other pathways should be accounted for. For example, PFAS mass that runs off or transfers to plants will not leach to groundwater. Thus, the mass losses (or mass loss rates) from runoff and plant uptake models could be subtracted from the total mass used in the leaching model. A similar accounting for loss from leaching could be included when estimating losses via runoff or uptake by plants. It may be necessary to run the models iteratively to obtain a reasonable mass balance between the model inputs (mass in) and outputs (mass out) between the respective models. If there is significant uncertainty regarding the mass loss rates or mechanisms, then the losses from one pathway may be ignored when modeling another pathway(s).

If the models reviewed herein are used to derive allowable concentrations of PFAS in amended soils, many of the parameters listed above would also need to be considered. For a specific site, they would be much the same as those used to predict concentrations migrating off site. For generic application, such as developing allowable concentrations for a larger geographic area (such as a state), the assumptions would likely be representative of generic or default conditions.

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Given the variability of individual PFAS transport behavior and toxicity, PFAS should not be treated as a single class when predicting behavior in models or in setting regulatory targets.

1.3 Model Screening and Review

Numerous models have been developed over the last several decades to evaluate leaching to groundwater, constituent runoff, and (to a lesser extent) plant uptake. These models were identified by reviewing compilations from the United States Environmental Protection Agency (USEPA) and the U.S. Geological Survey (USGS), as well as by conducting an online search for models used in North America. Analytical (mathematical) and numerical models were considered. A list of all the models identified during this review is included in Appendix A (Tables A-1 through A-3). Although this list is not exhaustive, it is extensive and captures the more commonly used models in North America. Due to the large number of models identified, a multi-step process was used to screen out and assess the available models and their potential suitability for PFAS modeling.

First, models were screened based on their status and overall suitability for PFAS modeling. This was a high-level screening focusing on the following criteria: 1) the intended application of the model (can it be used for constituents like PFAS?), 2) peer review status (has the model been peer reviewed?), 3) availability/support (is the model updated or supported?), and 4) availability/accessibility of the model (is the model available in the public domain or is it proprietary software?). In general, models were selected for further review if they met all criteria; the models are maintained (updated/revised), commonly used in the industry, designed for use for a variety of scenarios (e.g., not designed solely for landfills or as a regional screening model), and/or used input parameters that could be modified to simulate PFAS transport (e.g., sorption). During the initial screening step, each transport pathway was evaluated separately, as some factors were unique to each pathway. Appendix A summarizes the results of the initial model screening for the three respective pathways (Tables A-1, A-2, and A-3).

The retained models were evaluated further to assess their suitability to simulate PFAS transport as well as their relative advantages and disadvantages. These technical merits and capabilities were considered in determining if the models are suitable for PFAS modeling and screening assessments. The key parameters for PFAS modeling are summarized in Table 1. Tables 2, 3, and 4 summarize the model reviews for leaching to groundwater pathways, surface water runoff, and plant uptake, respectively. For the plant uptake pathway, screening and review were integrated and are summarized in Table 4. The models for the three pathways are described below in further detail.

2 LEACHING MODEL REVIEW

Numerous leaching models are available for a wide range of organic and inorganic constituents, but no models have been developed specifically to address PFAS leaching. The objective of this model review is to evaluate existing vadose zone leaching models for their ability to simulate PFAS leaching in the vadose zone to groundwater. Groundwater fate and transport was not evaluated. However, some of the models are capable of simulating groundwater flow (e.g., MODFLOW-USG/MT3D) or approximating groundwater fate and transport (e.g., SEVIEW). As described in Section 1.2, a stepwise approach was followed to screen out models that either are no longer used in the industry or could not be used for PFAS. Next, the retained models were evaluated based on their ability to account for the unique physicochemical characteristics of PFAS and to model the key leaching mechanisms. The key leaching mechanisms and parameters for PFAS are summarized below, and the selected models and review are discussed in Section 2.2.

2.1 Leaching Mechanisms

Vadose-zone systems are complex, involving the interaction of air, solids, and water under variably saturated conditions. Understanding vadose-zone transport and leaching mechanisms is crucial for modeling fate and transport of constituents, as they leach from areas of elevated concentration and percolate downward to groundwater. Various climate, physical, chemical, and biological factors control the movement of PFAS through the subsurface including recharge, advection, dispersion, diffusion, sorption, air-water interface partitioning, electrochemical interactions, volatilization, and degradation mechanisms. The more important mechanisms to PFAS leaching fate and transport are described briefly below.

2.1.1 Recharge and Advection

This mechanism occurs when precipitation and/or irrigation water percolates from the soil surface into the soil and the constituents are carried in the percolating water through the vadose zone to groundwater. This is the primary mechanism of PFAS leaching. Infiltrating water is also directly related to the relative soil permeability and the water saturation that affect all other PFAS transport mechanisms.

2.1.2 Dispersion and Diffusion

This mechanism is a function of the overall water content and pore size distribution. Diffusion and dispersion effects on the fate and transport of PFAS are considered moderate to minor compared to the other parameters that affect modeling of PFAS leaching.

2.1.3 Hydrophobic Sorption (K_{oc})

Sorption is a function of the constituent adsorption-desorption distribution coefficient (K_d), soil composition (e.g., clay content), organic carbon, and surface area. For most organic compounds, including PFAS, the K_d is generally controlled and predicted by the product of the K_{oc} and the fraction of organic carbon (f_{oc}) of soil (hydrophobic sorption). For PFAS with lower K_{oc} values (e.g., shorter-chain PFAS), binding by electrostatic attraction or air-water interface partitioning may be more influential on K_d (see below) than

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hydrophobic sorption. Sorption and desorption are generally assumed to be linear and collectively act to retard (slow down) chemical transport. However, desorption rates are often slower than sorption rates and/or are incomplete (i.e., only a portion of the sorbed mass desorbs). A 2019 study indicated that sorption/desorption rates for PFOS were non-ideal (i.e., desorption rates were not the same as sorption rates and behaved in a non-linear manner), and that additional pore flushes may be necessary to reduce PFOS (and likely PFAS) concentrations in porewater (Brusseau et al. 2019b). This may be attributed in part to electrostatic binding and air-water interface partitioning (see below). Sorption is considered an important factor when modeling PFAS leaching. For more accurate modeling results, a dual domain, non-linear isotherm model may be necessary (Brusseau et al. 2019a).

2.1.4 Air-water interface partitioning (K_{ia})

This mechanism occurs when constituents preferentially align themselves along the interface between porewater and air. PFAS tend to align themselves at such interfaces, with their perfluoroalkyl tails in the air phase and their ionic functional groups in the water phase. This tendency leads to storage at the air-water interfaces present in partially wetted pore spaces. Because the vadose zone is characterized by variable saturation (water and air), this is expected to be moderately important in PFAS vadose-zone modeling, particularly for PFAS that have lower K_{oc} values or when carbon concentrations in soils are lower. The leaching models identified and evaluated in this report did not have this capability. A study by Lyu et al. (2018) and Guo et al. (2020) indicated this parameter is critical for leaching models. The additional effects of K_{ia} on the overall retardation of PFAS may be accounted for using an approach outlined by (Lyu et al. 2018 and Guo et al. 2020). However, this effect in the vadose zone is reported to be concentration dependent (Guo et al. 2020) and may not be significant for low concentrations of PFAS. Further research and model development are needed in this area for PFAS leaching.

2.1.5 Electrostatic Adsorption

This mechanism occurs when negatively or positively charged constituents (or polar ends) bond with oppositely charged ions in soils (e.g., cations bonding to negatively charged clays in the vadose zone). A few of the leaching models identified and evaluated in this study have this capability. Electrostatic adsorption can be included in the K_d term to account for electrostatic adsorption's contribution to retardation. However, nearly all of the models have the ability to evaluate the net effects of retardation through the use of K_d . Further research and model development may be needed in this area for PFAS leaching, if this type of adsorption is non-ideal.

2.1.6 Surfactant-induced Flow

This mechanism occurs when the surfactant properties reduce surface tension of the water-air-soil interface thereby inducing vertical porewater flow in the subsurface. Surfactant-induced porewater flow is concentration dependent and may influence porewater flow and ultimately transport in the vadose zone if the PFAS porewater concentrations are elevated (Guo et al. 2020).

2.1.7 Volatilization

Volatilization is a function of chemical volatility (Henry's Constant, K_h) and interconnected unsaturated (air) porosity. Some PFAS constituents are moderately to slightly volatile (e.g., fluorotelemer alcohols [FTOHs]), while others exhibit negligible volatility. Thus, volatility may need to be considered for longer-term vadose-zone fate and transport assessments for the more volatile PFAS constituents.

2.1.8 Degradation

This mechanism occurs abiotically or biotically. PFAAs are considered persistent because they are stable and generally do not naturally degrade. PFAA precursor transformation to other PFAS in the environment, especially to PFAA, also may need to be considered. Precursor transformation can be conservatively evaluated by summing the precursors and their likely terminal daughter products for a more conservative assessment. Typically, only a portion of the precursors will convert to PFAA daughter products, and this should be assessed based on available scientific information and/or as described in Section 1.2.2.

2.1.9 Summary and Considerations

The key parameters for PFAS vadose-zone fate and transport modeling include: source area terms (finite or infinite sources), infiltration rate(s), sorption, air-water interface partitioning, dual domain, advection/dispersion (for larger scales), and volatilization (for the more volatile PFAS constituents). Therefore, models and/or the input assumptions used should consider these factors.

The dual-domain mass transfer approach for solute transport modeling is a method to represent the effects of heterogeneous advection and diffusive mass storage. The soil is divided into two compartments: a mobile domain where advection dominates and an immobile domain where mass storage dominates. Mass is transferred between compartments based on concentration differences and a constant, which is affected by groundwater flow, soil heterogeneities, and solute diffusion.

In some cases, the sorption terms (like air-water interface partitioning, electrostatic attraction, and dual domain effects) can be combined into a single sorption (K_d) term. However, this will generally be conservative and less accurate because it will assume that desorption rates are the same as sorption rates, resulting in more rapid and elevated peak concentrations at the discharge boundary to groundwater than is expected for PFAS in the vadose zone.

2.2 Review of Selected Leaching Models

A large number of leaching models have been developed over the past several decades to model the fate and transport of a wide range of constituents through the vadose zone. The leaching models retained and discussed in this report focus on numerical models used over the last one to two decades that are capable of steady-state and transient simulations. Thirty-two models were identified and are summarized in Appendix A. Eighteen leaching models retained after the initial screening were further reviewed for applicability to modeling PFAS leaching. Table 2 summarizes the details of the 18 retained models, along with their advantages and disadvantages for modeling PFAS leaching.

Three models were identified as having the potential to model PFAS leaching in the vadose zone (Table 2). All three models discussed below have the capability to model: sorption (via soil-water partitioning)

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using more than one isotherm, ion exchange, and volatilization. All three are numerical models and rely on standard advection-dispersion equations and Richard's equation (model) for variably saturated conditions (i.e., vadose zone).

2.2.1 HYDRUS 1D, 2D, and 3D

HYDRUS is a widely used software program by PC Progress that numerically models' water and solute movement through unsaturated, partially saturated, or saturated zones (Simunek et al. 2009). HYDRUS is available in one-dimensional (HYDRUS 1D), two-dimensional (HYDRUS 2D), and three-dimensional (HYDRUS 3D) formats. HYDRUS 1D is publicly available and free, while HYDRUS 2D and HYDRUS 3D are available for licensing fees that vary depending on which domain type is required. Additional modules may also be required for more complex chemical transport mechanisms at an added cost.

HYDRUS allows for the simultaneous transport of multiple solutes. The flow equation can incorporate a dual-porosity (or dual-permeability) flow model. The flow equation can also account for root-zone water uptake by plants using a sink term and can account for root growth using a logistic growth function. HYDRUS allows the user to specify various soil properties, and the flow region may comprise nonuniform soils. Head and flux boundaries are controlled by user-specified atmospheric conditions (e.g., precipitation), and free drainage can be applied as a boundary condition. The user can incorporate changes in boundary conditions during the simulation (i.e., soil surface boundary conditions can change from prescribed flux to prescribed head and vice versa, if needed). Unsaturated soil hydraulic properties are described using van Genuchten (1980), Brooks and Corey (1964), and modified van Genuchten type analytical functions. Hysteresis is incorporated into HYDRUS using the models introduced by Scott et al. (1983) and Kool and Parker (1987). In solute transport, the advection-dispersion equations in HYDRUS account for transport in both liquid and gaseous phases. HYDRUS also has options for modeling nonlinear or nonequilibrium reactions between soil and water, linear equilibrium reactions between soil and vapor, zero order production, and first-order degradation reactions. The degradation reactions can either be independent of other solutes or consider coupling between solutes in sequential first-order decay reactions. Flow and transport can occur in the vertical, horizontal, or inclined directions (for 2D and 3D versions).

Add-on modules are available to allow for additional specialized modeling such as 2D transport and reactions of major ions, reactions in 2D constructed wetlands, dual-permeability transport (i.e., preferential and nonequilibrium flow and solute transport), 2D colloidal facilitated transport, and coupled modeling with PHREEQC geochemical code (to consider mixed equilibrium and biogeochemical reactions). These add-on modules can be used to account for some of the fate and transport mechanisms that are assumed to have a relatively small effect on PFAS leaching (e.g., ionic bonding) compared to mechanisms that are known to have a substantial effect (e.g., sorption/desorption). HYDRUS has detailed documentation and training modules to support the application of the program and is regularly updated and maintained. The GUI allows for easier use of the program and permits user-defined inputs of key modeling parameters for PFAS transport.

For PFAS modeling, HYDRUS 1D models most of the key PFAS parameters identified in Sections 1.2 and 2.1, is widely used and accepted in the industry, is well supported (ample documentation and regularly updated) and is available for free. If enhanced model capabilities are needed, then HYDRUS 2D and 3D, as well as add-on modules, are available for a fee.

2.2.2 HYDROGEOCHEM 4.0/5.0

HYDROGEOCHEM is a numerical model by Scientific Software Group that iteratively solves problems of fluid flow, hydrologic transport, and biogeochemical reactions in variably saturated media in both two dimensions (Version 4.0) and three dimensions (Version 5.0; Scientific Software Group 2019). Both HYDROGEOCHEM Versions 4 and Version 5 are available for a licensing fee.

HYDROGEOCHEM is designed for generic applications of reactive transport problems controlled by both kinetic and equilibrium reactions in the subsurface (Oak Ridge National Laboratory 2004).

HYDROGEOCHEM can simulate the reactive transport of multiple chemical constituents in the subsurface under variably saturated conditions. HYDROGEOCHEM computes and predicts the distribution of pressure head, moisture content, flow velocity, total head, and spatial-temporal distribution of chemical constituents over a two- or three-dimensional plane in unsaturated or saturated media. The model considers slight deformation of the media, pressure and gravity forces, capillary tension, evaporation, transpiration, infiltration, and artificial injection and pumping. The reactive solute transport results consider the geochemical equilibrium of aqueous reactions, including complexation, reduction-oxidation, sorption (including surface complexation, constant capacitance, and double-layer approaches), ion exchange, acid-base reactions, precipitation, and dissolution. Solute transport also considers the effects of hydrological transport, including advection, dispersion, and the effects of unsaturation.

HYDROGEOCHEM is a widely used and accepted modeling program that is supported and maintained. For PFAS modeling, the advantages of HYDROGEOCHEM are that it has a good GUI and allows flexibility for user-defined input parameters for aquifer characteristics such as lithologic layers. It also models most key PFAS parameters. However, application of HYDROGEOCHEM is limited to single-porosity media (dual-porosity media cannot be effectively modeled). Additionally, site-specific modeling of some of the less critical PFAS parameters (e.g., electrostatic bonding) would require costly add-on packages.

2.2.3 SVENVIRO™ (formerly SVCHEM and SVFLUX)

SVENVIRO™, which combines SVFLUX™ with the software formerly called SVCHEM™ and is environmental fate and transport modeling software available for a fee by Bentley Systems. SVFLUX™ models groundwater seepage in unsaturated or saturated soils and rock. It is offered as a 1D, 2D, and 3D finite-element program for simulating steady-state and transient-state groundwater flow. SVENVIRO™ is capable of modeling sites with complex water flow and solute transport pathways, including coupled water flow, freeze/thaw analysis, and pore-air flow models. The analysis includes a comprehensive climatic interface. SVENVIRO™ solves the flow and transport equation using the finite element method, and the model can couple saturated and unsaturated flow. The software features fully automatic mesh generation and mesh refinement in 1D, 2D, and 3D models (Soil Systems Limited 2019a and 2019b). SVENVIRO™ incorporates climate boundary conditions including evaporation, transpiration, snow, and energy balance, and the software can incorporate site-specific weather station data. The transport model incorporates terms for advection, dispersion, diffusion, absorption, and biological and radioactive decay.

The processes of SVENVIRO™ can evaluate groundwater flow and pore-vapor flow equations either independently or as coupled processes. Add-on programs (i.e., SVDESIGNER™) allow the user to create geometrically complex digital models. The model can incorporate multiple layers with different geometries and soil properties (including layers that pinch out).

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SVENVIRO™ is an industry-accepted model that is regularly maintained and supported. For PFAS modeling, the advantages of SVENVIRO™ are the sophisticated 3D model construction capabilities, particularly the ability to model layers with different geometries and soil properties (including layers that pinch out). However, the inability to model dual domain may partially limit its ability to model PFAS transport accurately. The GUI (a CAD-based front end) and automated solver are intuitive to use, and training and support are offered by Bentley Systems at additional cost.

2.3 Leaching Model Summary and Recommendations

Three models were identified as having the potential to model PFAS leaching (in alpha-numeric order):

- Hydrogeochem (4.0/5.0)
- Hydrus (1D, 2D, and 3D)
- SVENVIRO™.

These three models are robust, well maintained, well documented/reviewed, and are the most likely to be updated to adopt additional, key PFAS modeling parameters like K_{ia} . However, none of the models reviewed are able to model all of the key parameters that affect PFAS leaching from land applied residuals. In particular, none of the models reviewed has the capability to model air-water interface partitioning. Because air-water partitioning, when present, is assumed to act as a mechanism that retards transport and acts to limit the mass of PFAS available to leach from land-applied residuals in the vadose zone, the inability of these models to account for such partitioning and retardation is likely to result in the models overestimating, rather than underestimating, the concentration of PFAS in leachate. A lower retardation rate would result in higher PFAS transport velocities, reducing the time it would take to reach groundwater and overestimating the loading rate to groundwater. Such overestimates of PFAS loading rates may be acceptable depending upon the purpose of the application of the models (e.g., developing conservative estimates of PFAS concentrations in leachate). Additional research will likely be necessary to understand how accurately the existing models are able to simulate PFAS leaching, whether additional model development may be necessary to improve predictive ability, and the degree of improvement in predictions such additional development is likely to garner. Key input and output parameters for these models are presented in Exhibit 4.

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Exhibit 4. Key Input and Output Parameters for Leaching Pathway Models

Model	Key Input Parameters	Key Output Parameters
Hydrogeochem (4.0/5.0)	<ul style="list-style-type: none"> • <i>Model Domain Parameters</i> – mesh size and number of nodes, time steps • <i>Media/Flow Properties</i> - advection and dispersion coefficients, hydraulic conductivity and permeability, flow velocity, moisture content • <i>Reaction Properties</i> – Initial solute concentrations, sorption coefficient (K_d) • <i>Boundary Conditions</i> – Constant head, variable flux, gradient flux, reservoir 	<ul style="list-style-type: none"> • Pressure head and total head • Velocity fields • Moisture content • Biogeochemical concentrations (as a function of time and spatial distribution) • Particle flow (2D and 3D)
Hydrus (1D, 2D, and 3D)	<ul style="list-style-type: none"> • <i>Model Domain Parameters</i> – mesh size and number of nodes, time steps • <i>Media/Flow Properties</i> - advection and dispersion coefficients, hydraulic conductivity and permeability, flow velocity, moisture content, optional dual porosity (domain)*, optional root water uptake*, optional PHREEQC link* • <i>Reaction Properties</i> – Solute concentrations, sorption coefficient (K_d) • <i>Boundary Conditions</i> - Constant head, variable flow & solute flux, and gradient flux. Solute transport boundaries also allowed. 	<ul style="list-style-type: none"> • Mean pressure head • Mean and cumulative water flux • Mean and cumulative solute concentrations (as a function of time and spatial distribution), mean and cumulative solute flux • Particle flow (2D and 3D)
SVENVIRO™	<ul style="list-style-type: none"> • <i>Model Domain Parameters</i> – mesh size and number of nodes, time steps • <i>Media/Flow Properties</i> - advection and dispersion coefficients, hydraulic conductivity and permeability, flow velocity, moisture content • <i>Reaction Properties</i> - Sorption coefficient (K_d; including user defined sorption isotherms) • <i>Boundary Conditions</i> - Constant head, variable flux, or gradient flux 	<ul style="list-style-type: none"> • Pressure head and total head • Linear velocity • Moisture content • Biogeochemical concentrations (as a function of time and spatial distribution)

Notes:

Flux terms (like flow and mass) are a function of time. Generally moisture content is also a function of time in transient models. Table based on readily available literature. Actual model inputs and outputs may vary.

* = unique/advantage

Seven additional vadose-zone models were identified that may be used to model PFAS, assuming that their respective limitations are accounted for and include:

- MT3D-USGS/MODFLOW-USG
- PWC/PRZM5
- SEVIEW/SESOIL
- Source Screening Module (SSM)
- STANMOD

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- TOUGH3
- VS2DI.

These models were screened out either because they were too complex to use (MT3D-USGS and Tough3), lacked key modeling capabilities (SSM, MT3D-USGS/MODFLOW-US,G and VS2DI), and/or had documented limitations (SEVIEW) as summarized in Table 2. PWC/PRZM5, SSM, and SEVIEW are better suited for screening-level assessments. For example, PRZM5 has been used as a screening tool in the Northeastern U.S. to estimate the leaching potential of select PFAS. The remaining leaching models reviewed are generally considered unsuitable or less suitable for PFAS modeling as indicated in Appendix A and Table 2.

3 SURFACE WATER RUNOFF MODEL REVIEW

PFAS transport from residual land applications may occur through runoff to surface water bodies. As PFAS are an emerging group of compounds with complex physiochemical behaviors, a modeling structure for predicting PFAS concentrations in runoff has yet to be developed. There are currently several commonly used runoff models that address transport of constituents on both a watershed and local (field) scale. However, due to the unique chemistry of PFAS and the mechanism of PFAS introduction to the environment (i.e., land application of residuals), it is not clear if existing models may appropriately model PFAS transport through runoff. The objective of this model review was to evaluate existing runoff models and determine if they are applicable to modeling PFAS transport via runoff. A list of commonly used and/or widely available runoff models was developed and reviewed to determine if model inputs and equations could accurately model PFAS behavior. As described in Section 1.2, a stepwise approach was followed to screen out models that either are no longer used in the industry or are not applicable to modeling PFAS. Following an initial screening step, the retained models were further evaluated based on their ability to account for some of the unique physicochemical characteristics of PFAS. The key runoff mechanisms and parameters for PFAS are summarized in Section 3.1, and the models considered suitable for modeling PFAS are discussed in Section 3.3.

3.1 Runoff Mechanisms

When precipitation does not infiltrate through soil, it runs across the soil surface and may enter surface water bodies such as streams, lakes, and rivers (USGS 2019). Surface water runoff is the component of the hydrological cycle that enables precipitation to carry soils, sediments, chemicals, and nutrients to surface waters. The amount of surface water runoff that may replenish surface water bodies is affected by several physical properties of the land and metrological characteristics. Topography, land cover (vegetation type), and soil properties, along with the amount of precipitation and the duration and intensity of a storm event, all control the amount of potential runoff (Yang et al. 2015). When the intensity of a storm exceeds the rate at which water can infiltrate into a specific soil class, or when the maximum water holding capacity of the soil has been reached, precipitation will run off the land on which it fell and may reach a surface water (Yang et al. 2015).

The fate and transport of constituents in runoff is dependent on the physical, metrological, chemical, and biological properties of a site, soil, and constituent. Air-water interface partitioning (Henry's law constant), solubility, volatilization, sorption/adsorption, degradation mechanisms, and transformation rates all affect how readily a constituent may move in runoff. Runoff models must consider all of these properties to evaluate the transport of constituents into surface waters. For PFAS, soil sorption (K_{oc}), air-water interface partitioning, transformation rates, and electrostatic adsorption (K_d) are the key parameters for transport through runoff.

3.1.1 Hydrophobic Sorption (K_{oc})

In general, the organic carbon water equilibrium partitioning constant (K_{oc}) increases as perfluoroalkyl chain length increases, although PFBA has a higher K_{oc} than PFPeA (Guelfo et al. 2013, Anderson et al. 2019). The tendency of PFAS to adsorb to soil organic matter will impede their mobility in a dissolved aqueous form. The soil-water partitioning coefficient (K_d) for hydrophobic organic compounds is the product of K_{oc} and the fraction of soil organic carbon (f_{oc}). Substantial data on empirical K_{oc} values are available for PFAA, while few data are available for PFAA precursors (Guelfo et al. 2013, Anderson et al. 2019).

3.1.2 Air-Water Interface Partitioning (K_{ia})

PFAS have a tendency to align themselves at the surfaces of air-water interfaces, with their perfluoroalkyl tails in the air phase and their ionic functional groups in the water phase. This tendency leads to storage at the air-water interfaces present in partially wetted pore spaces. This partitioning phenomenon can be expressed by an air water interface partitioning coefficient, or K_{ia} . The saturation of residuals applied to soil or of soil into which residuals have been mixed, can affect the availability of PFAS for transport in runoff. Because of this phenomenon, dry residuals may have a lower contribution of PFAS to runoff than wet residuals (Brusseau 2018, Lyu et al. 2018).

3.1.3 Electrostatic Adsorption (K_d)

Electrostatic-based adsorption (K_d) is dependent on soil composition and pH as well as the individual PFAS structure. Hydrophobic adsorption (K_{oc}) is the main mechanism by which PFAS are retained in soils (Guelfo et al. 2013, Higgins and Luthy 2006, Barzen-Hanson et al. 2017, Anderson et al. 2019); however, electrostatic processes can be a significant retention process for positively charged polyfluorinated PFAA precursors (Mejia Avendano et al 2017, Barzen-Hanson et al. 2017).

3.1.4 Transformation Rates

PFAA do not transform in the environment; however, PFAA precursors (i.e., polyfluorinated compounds) may be present in residuals and can slowly transform through microbial processes. Precursors transform more rapidly under aerobic conditions than anaerobic conditions (Zhang et al. 2013, Zhang et al. 2016, Yi et al. 2018). Additionally, terminal PFAA products have only been observed to form under aerobic conditions, while intermediate polyfluorinated products form under anaerobic conditions. The presence of these precursors, and their subsequent transformation, may increase the amount of PFAA in residuals and/or runoff water. Typically, only a portion of the precursors will convert to PFAA daughter products, and this should be assessed based on available scientific information and/or as described in Section 1.2.2.

3.2 Review of Selected Runoff Models

A large number of runoff models have been developed over the past several decades to evaluate runoff. Thirty models were identified during the initial review. As described in Section 1.2, a stepwise approach was followed to screen out models that either are no longer used in the industry or could not be used for evaluating PFAS in runoff. For the initial screening, the intended application of the runoff model included model rejections if the model was only applicable to a certain land cover type, if the model only accounted for the amount of runoff but not the concentration of a constituent in runoff, if no chemical application could be input for the model, or if the model scale was too large. Ideally, a field-scale model would represent the runoff scenario best. The results of which are summarized in Appendix A Table A-2. Three of the 30 potential runoff models were retained for additional evaluation and included:

- Multimedia, Multi-pathway, Multi-receptor Exposure and Risk Assessment (3MRA)
- Pesticide in Water Calculator (PWC)
- Water, Energy, and Biogeochemical Model (WEBMOD).

The three retained models were evaluated further based on their ability to account for the unique physicochemical characteristics of PFAS and to model the key runoff mechanisms, the scale of the model (field/watershed/landfill/urban drainage), and PFAS runoff mechanism. While some models were rejected in the initial screening due to the scale of the model, two models were further reviewed that were on a watershed scale to determine if outputs from isolated applications to a field or near a stream within the model framework may allow for the prediction of concentrations in runoff. Table A-2 summarizes the details of each of these models, along with their advantages and disadvantages for modeling PFAS in runoff.

The two initial model screening and evaluation steps found that, while several runoff models have been developed to model hydrological processes on a watershed scale in both urban and rural landscapes, many of these runoff models do not simulate constituent transport in runoff at a field scale, where site-specific and chemical-specific parameters can be incorporated. PWC appeared to be the most suitable model to evaluate PFAS transport in runoff.

PWC was designed to estimate pesticide concentrations in surface water and groundwater resulting from agricultural applications of pesticides, but also can be used for other constituents. PWC simulates both surface and groundwater and is composed of a field model (PRZM 5) and a water body model (VVWM 1; USEPA 2016). PWC is a commonly used model that is routinely updated and maintained by the USEPA. PWC is available online for free download. PWC's PRZM 5, Variable Volume Water Model (VVWM), and inputs are summarized in the following sections, respectively.

3.2.1 Pesticide in Water Calculator – PRZM5

PRZM5 simulates chemical changes to mass in the soil primarily by runoff, erosion, volatilization, leaching, and degradation. The hydrological component of the model calculates both runoff and erosion based on the Soil Conservation Service Curve Number (CN) method and the Universal Soil Loss Equation. Water balances are maintained for runoff, evapotranspiration, temperature, irrigation, and precipitation from site-

specific model inputs. Movement of water through the soil profile is simulated by a capacity model and is dependent upon soil field capacity and wilting point. PRZM5 models runoff as a portion that interacts with soil and a portion that does not. Where runoff interacts with soil, it conceptually has a flow profile that decreases exponentially as depth increases. Therefore, PRZM5 maintains equilibrium conditions between runoff and soil. The dissolved, adsorbed, and vapor-phase concentrations of constituents in soil are calculated through the processes of runoff, erosion, degradation, volatilization, foliar wash off, plant uptake, leaching, dispersion, and sorption on a daily time step (Young and Fry 2016).

Additionally, PRZM5 can handle nonlinear isotherms and nonequilibrium sorption. PRZM5 allows the specification of sub-daily time steps to avoid numerical issues. With a sub-daily time-step, the hydrologic calculations, such as runoff, are a direct fraction of the total daily flow that are in proportion to the time step and are not impacted by the sub-daily time step. The output is still recorded as a daily time step (Young and Fry 2016). Sorption in equilibrium and nonequilibrium regions is modeled with Freundlich isotherms, and the equilibrium region and nonequilibrium regions are solved by splitting the operations. Initially, the movement of the constituent from an equilibrium region to a nonequilibrium region is calculated from the analytical solution. Then, the advection dispersion degradation step is calculated numerically.

3.2.2 Pesticide in Water Calculator – Variable Volume Water Model

The Variable Volume Water Model (VVWM) is used to estimate pesticide exposure in surface waters as a result of agricultural applications to farm fields. VVWM also models the fate and transport of constituents in surface water bodies and the resulting estimated environmental concentrations. VVWM simulates standard water bodies defined by the USEPA (Index Reservoir scenario and USEPA Pond scenario) as well as user-defined water bodies. VVWM accounts for changes to several weather, hydrological, and chemical transformation parameters on a daily time step. These parameters include precipitation, temperature, windspeed, evaporation, water body volume, runoff, and pesticide dissipation (Young 2016).

3.2.3 Pesticide in Water Calculator Inputs

PWC includes a user-friendly graphical user interface (GUI) with tabs for all relevant input parameters needed for estimating PFAS concentrations in runoff. The “chemical” tab includes cells for the direct input of K_{oc} , f_{oc} , and K_d . In addition, there is the option to input chemical parameters for the parent and up to two additional daughter compounds.

The applications tab enables the entry of the number, method, and type of field applications based on a pre-defined scenario and a weather file. There are several diverse land application scenarios to choose from that reflect local crop-based agricultural practices and regional weather across the United States and Canada. In addition, scenarios continue to be developed by both the USEPA and Canada’s Pest Management Regulatory Agency (PMRA). Metadata files developed for each scenario are included with the free model download, so access to site-specific details is readily available. While the model does not currently include the option to select a residual application scenario, several existing application options would potentially be suitable for modeling of PFAS in land-applied residuals. The available crop/location

scenarios include options for Christmas trees and tree nurseries, which may be relevant surrogate scenarios for modeling residual applications to timber lands. The scenario and selected weather file are shown on the “crop/land” tab. Crop/land inputs also include site-specific soil horizon data to be entered including the number of soil horizons, their thickness, and the percentage of organic carbon in each interval, with the option to also simulate soil temperature. Input of site-specific soil horizon data is helpful, as so many of the critical parameters for modeling PFAS are dependent on site-specific soil characteristics.

The runoff tab is pre-populated by the designated weather file but also has parameters that can be adjusted by the user for the extraction of runoff and erosion. The simulation type, based on a predefined or user-defined water body, can be selected. The Farm Pond scenario is the most conservative, and the USEPA Reservoir scenario is less conservative. The Farm Pond scenario represents a farm pond on the edge of a treated field. The pond measures 1 hectare by 2 meters deep. For the farm pond, the inflow and evaporative losses are balanced, and leaching is not modeled (Young 2016). The USEPA Reservoir scenario represents a lake with perennial and ephemeral stream inputs. The flow into the lake can vary daily due to precipitation, evaporation, runoff, and groundwater discharge. The reservoir is simulated as a fixed volume where outflow is equated to the inflow of runoff to the lake (Young 2016). An option exists to perform batch runs with several scenario types and tabs for model outputs depending on the waterbody scenarios specified. Most relevant to the purposes of predicting PFAS concentration in runoff, the output tabs include the concentrations of the relative transport of runoff. Runoff is reported as the overall fraction of the total mass that was transported to the water body. In addition, the water column 1-in-10-year concentrations are also provided.

3.3 Runoff Model Summary

The initial runoff model screening consisted of a list of 30 potential models. Of the 30 models, three were deemed potentially applicable for PFAS modeling and were reviewed in more detail. Based on the more detailed review (Section 3.2), one model (PWC) was selected as the most applicable to modeling PFAS at a field scale, where direct applications can be made to a plot and runoff directly modeled. PWC was selected for its ability to model runoff as part of a water balance and as it interacts with soil (not just sheet flow as other models), for its range of landcover scenarios, the ability to enter site-specific weather data, and the applicable chemical-specific inputs that can be incorporated. In addition, transport-specific functions in the model handle complex nonlinear and nonequilibrium situations that may be exhibited by PFAS.

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Exhibit 5. Key Input and Output Parameters for Surface Water Runoff Model

Model	Key Input Parameters	Key Output Parameters
Pesticide in Water Calculator (PWC)	<ul style="list-style-type: none"> • <i>Flow</i>: Field application data, weather and irrigation data, soil characteristics (including thickness, bulk density, and runoff parameters (soil loss factors, curve number) • <i>Solute</i>: chemical parameters, including sorption coefficients (K_{oc} and K_d), and organic carbon content (f_{oc}), 	<ul style="list-style-type: none"> • Solute concentrations (as fraction of overall mass transported) • Water column and pore water concentrations (peak and average)

One of the limitations of PWC, and virtually all other models, is the inability to account for air-water interface partitioning (K_{ia}) and the surface tension effects. While it is unclear exactly how K_{ia} and the surface tension effects of PFAS will affect surface water runoff from land-applied residuals, it is expected to be relatively minor because air-water interfaces in surface water runoff are minimal.

4 PLANT UPTAKE MODEL REVIEW

PFAS in soil and/or groundwater can enter the food chain through uptake by plants. Several plant uptake models are available for a wide range of organic compounds, though none of these models has been exclusively developed for PFAS. Additionally, studies have investigated plant uptake of PFAS from residuals-amended soil in various crops. One objective of this section is to review the available plant uptake models and discuss their suitability to model uptake of PFAS from residual-amended soils. A second objective of this section is to review readily available literature-based soil to plant transfer factors for PFAS.

4.1 Plant Uptake and Loss Mechanisms

In general, the uptake of chemicals by plants is governed by the following processes:

- Desorption from soil followed by root uptake from soil solution
- Direct contact between soil and plant tissue
- Transport in the transpiration stream
- Gaseous and particulate deposition to aboveground plant parts.

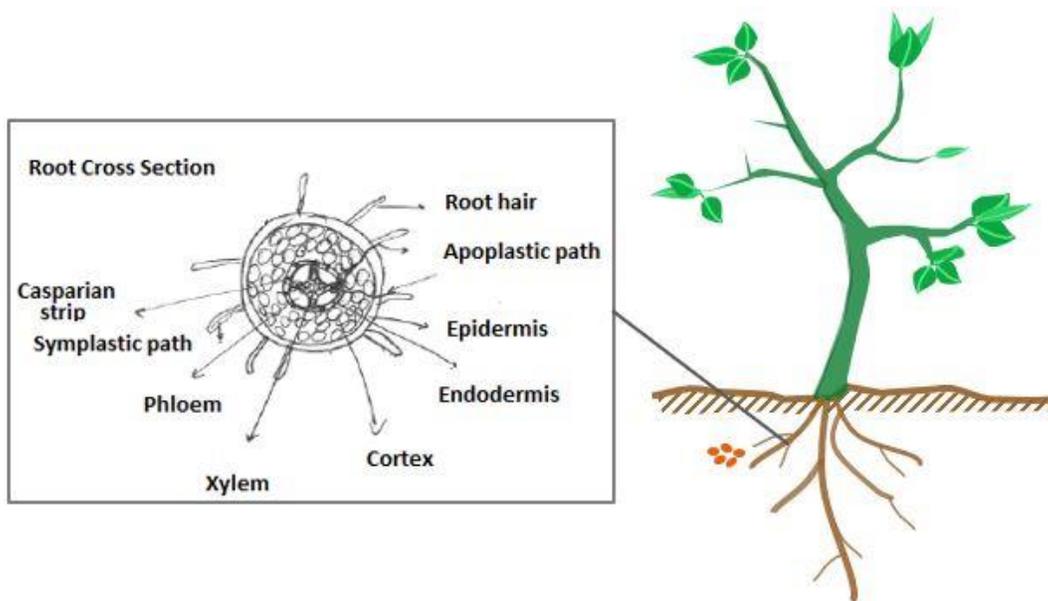
The translocation and partitioning behaviors of chemicals in plants are complex and depend on both chemical properties and plant characteristics. The basic pathways governing chemical uptake by plants are well known and are briefly summarized below. Evaporation and volatilization from leaves as well as metabolism and growth dilution are considered loss mechanisms and are discussed in Section 4.1.5.

4.1.1 Root Uptake

Organic chemicals are taken up from both water and air via plant roots. Uptake includes passive (diffusive) and active processes. Chemicals are taken up by plants through passive processes during transpiration. Active absorption occurs by absorption of water through plant root hairs via osmosis. Water moves from plant hair roots to the plant via a symplast pathway from cell to cell. Neutral chemicals will first reach equilibrium between the soil solution and plant roots and then sorb to lipophilic solids including lipids in membrane and cell walls within the root system (Martin et al. 2006). A generic term called “the root concentration factor” is defined as the ratio of chemical concentration in the root to the corresponding concentration in soil porewater at equilibrium. The degree of sorption depends on both the hydrophobicity of the chemical as well as the amount of lipid in the root. Plant transpiration drives a passive transport mechanism (via diffusion) for the uptake of chemicals from porewater. This is a key process for neutral organic compounds. Root uptake of chemicals with high lipophilicity is lower than uptake of chemicals with low lipophilicity because chemicals with high lipophilicity have a lower concentration in porewater and they compete for sorption between plant lipids and soil organic carbon resulting in a lower amount sorbed to plant roots.

A cross section of plant root is shown on Exhibit 6. Chemicals dissolved in the water flows across the root cortex and is transported via apoplastic and symplastic pathways until it arrives at the endodermis. The casparian strip is an endodermal cell wall of the plant root that acts as an ion trap for polar compounds. The ionized and neutral hydrophilic chemicals can pass through anion channels or water pores in the membrane, enter the transpiration stream, and move through various parts of plant (Blaine et al. 2014b). However, some ionized chemicals can be trapped in the membrane and prevented from passing pass through to the transpiration stream (Martin et al. 2006).

Exhibit 6. Conceptual Model of PFAS Uptake in a Plant



4.1.2 Transport from Roots to Other Plant Tissues

Water and other nutrients are transported via xylem from roots to other plant tissues including stems, leaves, tubers, and fruits. This process, known as translocation, is driven by transpiration. During transpiration, a mass gradient is created between the leaves and root system, causing the uptake of water through the root system that is transported to other plant tissues via the xylem. Phloem is responsible for the transfer of sucrose from leaves to other plant tissues such as fruits, tubers, and roots (Martin et al. 2006). Although the flow volume in xylem is reported to be 50 to 100 times greater than the flow volume in phloem, phloem is an important transport mechanism for ionized and polar chemicals with intermediate cell permeability ($\log K_{ow}$ of -0.47 or -0.57) (Bromilow and Chamberlain 1995).

Following vascular transport, water or solutes diffuse into and can be stored in adjacent plant tissue such as shoots, tubers, and fruits. The lipid composition of aboveground plant tissue plays an important role in the accumulation of non-ionized organic chemicals (Briggs et al. 1983). As discussed above, for ionized chemicals, the casparian strip between the root system and xylem controls the transfer of ionized species

within the plant tissues due to presence of protein in the cells. The degree of dissociation in plants may differ from the abiotic environment depending on the acidity or alkalinity levels of cells. The transport mechanisms controlling the uptake and fate and transport of ionized compounds in different parts of plants is poorly understood (Trapp 2003). Neutral and ionized polar chemicals with low lipophilicity and volatility, which are also resistant to biodegradation, are subject to accumulation in the aboveground compartments (e.g., leaves and fruits) through phloem transport. PFAAs, particularly the short-chain PFCA homologues, generally meet these characteristics and accumulate in aboveground compartments (Blaine et al. 2014b).

4.1.3 Vapor or Gas Uptake from Atmosphere

Uptake of chemicals from the vapor phase is an important mechanism for volatile chemicals and chemicals with greater tendency to partition to air than water. During this process, a chemical diffuses through the leaf and partitions to the aqueous or lipid phases of plant tissue. Examples of lipophilic leaf tissues include membranes, storage lipids, resins, surface lipids such as cutin, and cuticular waxes. Several studies have investigated the air-to-plant concentration factors for a variety of organic chemicals and their relationship to other physicochemical properties such as the octanol air partition coefficient (K_{OA}), Henry's Law constant, octanol water partition coefficient (K_{OW}), and molecular weight (Martin et al. 2006). The uptake of PFAA in soil through vapor phase is expected to be negligible because PFAS are generally not volatile and, if detected in the atmosphere, they are generally associated with particulate matter (Genualdi et al. 2010).

4.1.4 Particle Deposition on Plant Surface

The deposition of organic chemicals through wet or dry deposition of suspended particles on aboveground plant parts is an important transport mechanism for metals and radionuclides. Several factors govern the uptake of chemicals by plants following dry deposition of particles on the surface of a leaf include diffusion, interception, impaction, and sedimentation. Wet deposition involves the coagulation of solid particles with water droplets (Martin et al. 2006). The uptake via wet deposition is a function of leaf characteristics such as roughness, leaf wettability, and water storage capacity (Boyce et al. 1991). The uptake of ionized chemicals occurs mainly through the cuticle (Peuke et al. 1998). Currently, available information is insufficient on particle deposition mechanism(s) and how chemical properties affect uptake of chemicals from particles to leaves to estimate uptake of PFAA via particle deposition (Martin et al. 2006). However, this is expected to be a minor plant uptake pathway from PFAS in land-applied residuals given that the relative mass of PFAS in windblown particles from land-applied residuals is expected to be small compared to the relative mass in land-applied soils and available for root uptake.

4.1.5 Loss Mechanisms

Evaporation and volatilization through leaf-air exchange, metabolism, and growth dilution are the primary mechanisms by which the concentrations of chemicals in plants can be reduced. Information about PFAS loss mechanisms from plants is scarce. The rate of metabolism is plant- and chemical-specific. Limited

information is available on the metabolism of PFAS by plants, though Bizkarguenaga et al. (2016) have reported that some PFAS (e.g., PFOSA) can be metabolized and produce more stable PFAS compounds.

4.2 Review of Selected Plant Uptake Models

The plant uptake models discussed in this report have been published in peer-reviewed journals and have been developed based on either empirical data or mathematical modeling of uptake processes. A list of plant uptake models was published by USEPA and by the United Kingdom's Environment Agency. USEPA food chain and multimedia models available through the USEPA Centre for Exposure Assessment Modeling (CEAM) were reviewed to identify those with a soil-to-plant modeling component. Martin et al. (2006) reviewed plant uptake models to derive generic soil guidelines protective of human health from exposure to chemicals in soil via consumption of homegrown produce. A total of eight plant uptake models were identified and evaluated in Appendix A Table A-3 and summarized in Table 4.

Most of the mathematical and empirical models reviewed in this report assume chemicals are non-ionized and organic and that partitioning of chemicals in plants and the environment is primarily governed by their tendency to partition to carbon and lipids. Partitioning of PFAS is more complex and governed by additional physicochemical properties. Consequently, such models are unlikely to be applicable to estimating the accumulation of PFAS in plants from residual-amended soil. Mechanistic models developed for ionized chemicals could be applicable to PFAS (e.g., Gredelj et al. 2020). However, such models generally require substantial data, including PFAS-specific transfer factors, that may not be available for most PFAS. For this reason, using detailed mechanistic models for screening purposes is likely not practical at this time. Simple accumulation models in the form of literature-based soil-to-plant or solution-to-plant transfer factors are likely to be more appropriate for predicting the concentrations of PFAS in plants. A summary of readily available soil-to-plant transfer factors is presented in the next section and Appendix B.

4.3 Soil-to-Plant Transfer Factors for PFAS

Several studies have historically reviewed and compiled soil- or solution-to-plant uptake factors (referred to as transfer factors [TFs]) for PFAS. Newer studies refine the scientific understanding of TFs. A full description of the review and conclusions is provided in Appendix B. TFs from soil or solution to plants are available for diversity of plant species and tissue types and are summarized in Table B-1 (Appendix B).

For soil-to-plant TFs, two general, but not universally consistent, trends are apparent. The first is that TFs tend to decrease with increasing PFAS carbon chain length for all tissue types. This trend in TFs of PFAA is consistent with findings of other studies (e.g., Blaine et al. 2013, 2014; Krippner et al. 2015). The second trend is that soil-to-plant TFs for PFSA tend to be somewhat lower than TFs for PFCA in the same plant species and tissue type.

Three general, but not universal, trends are apparent for solution-to-plant TFs. First, solution-to-plant TFs for roots tend to increase with increasing carbon chain length; a trend that is the reverse of soil-to-plant TFs which decreased with increasing carbon chain length. Second, solution-to-plant TFs for fruits tend to

decrease with increasing carbon chain length; a trend that parallels that observed for of soil-to-plant TFs. Third, solution-to-plant TFs for fruits tend to be smaller than solution-to-plant TFs for roots.

4.4 Plant Uptake Summary

The review of plant uptake models indicates that most models have been developed for nonionized chemicals and rely on K_{ow} to estimate partitioning between water and carbon in soil and water and lipid in plants. Because partitioning of PFAS in many environmental settings is not predicted solely by K_{ow} , and once inside plants, PFAS partition to proteins as well as lipids, such models have limited ability to predict uptake of PFAS by plants. Mechanistic models developed for ionized chemicals have the potential to be relevant for PFAS (e.g., Trapp 2017; Gredelj et al. 2020). However, such models generally require substantial data, including plant-specific input parameters as well as PFAS-specific TFs, that are not currently available for most PFAS. For this reason, using detailed mechanistic models for screening purposes is likely not practical at present. However, developments associated with these types of mechanistic models are important to follow, as they could lead to a predictive capability in support of fate and transport modeling as they evolve. At present, simple bioaccumulation models in the form of literature-based soil-to-plant or solution-to-plant TFs are more appropriate for predicting the concentrations of PFAS in plants.

A compilation of literature-based soil-to-plant and solution-to-plant TFs for PFAS is presented in Table B-1 from the reviewed publications where available. TFs were compiled for the six edible crop categories shown below as well as vegetative parts of crops where available (Table B-1).

- Root vegetables: radish (root), carrot (total and core), potato (tuber)
- Leafy greens: cabbage (head), lettuce (leaf, total), spinach (total)
- Fruits: strawberry (fruit)
- Animal feed: maize (stover, straw), wheat (shoot, husk), spring wheat (straw), rapeseed (shoot), oat (straw), alfalfa (shoot), ryegrass (shoot), grass
- Legumes and grains: spring wheat (grain), wheat (grain), maize (grain), mung bean (shoot), soybean (shoot), pea (fruit)
- Other vegetables: zucchini (fruit), tomato (fruit), celery (shoot), pumpkin (shoot), rapeseed (plant), alfalfa (shoot), cucumber (fruit).

While no formal data analysis of TFs summarized in Table B-1 was conducted, some general but not universally consistent trends in soil-to-plant TFs are apparent including:

- Soil-to-plant TFs tend to decrease with increasing PFAS carbon chain length for all tissue types
- Soil-to-plant TFs for PFSA tend to be somewhat lower than TFs for PFCA in the same plant species and tissue type
- Solution-to-plant TFs for roots tend to increase with increasing carbon chain length

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- Solution-to-plant TFs for fruits tend to decrease with increasing carbon chain length
- Solution-to-plant TFs for fruits tend to be smaller than solution-to-plant TFs for roots.

The TFs provided in the literature were mostly reported as the ratio of the concentration of PFAS in paired plant tissue and soil (or solution) samples and are not based on regression analysis of changes in PFAS concentration in plant tissue across a range of soil or solution concentrations. A more robust understanding and representation of PFAS accumulation in plants could be developed using regression analysis, assuming suitable paired soil (or solution) and plant data are available.

In summary, the compilation presented in Table B-1 presents available TFs for many common crop species and can be used to estimate uptake of several PFAS by a range of plant species. The compilation can also be used to identify additional data needs and research priorities to enhance the understanding of the factors that affect the accumulation of PFAS including different soil characteristics, different plant species and tissues, and varying PFAS characteristics (e.g., chain length and functional groups).

5 SUMMARY AND CONCLUSIONS

PFAS transport mechanisms are relatively complex compared to other historically modeled constituents of concern in residuals (e.g., trihalomethanes, dioxins/furans, metals). The following model input parameters are considered important to reliable PFAS modeling:

- Hydrophobic adsorption and desorption
- Soil-to-plant bioaccumulation and TFs
- PFAA generation from precursors
- Air-water interface partitioning
- Electrostatic adsorption.

These parameters carry varying importance for the respective transport pathways as indicated in Exhibit 1 and detailed in Table 1.

Seventy models were identified for modeling PFAS leaching to groundwater, runoff in surface water, and/or plant uptake. However, only a handful of models were identified that are considered suitable for modeling PFAS, and no single model was identified for modeling all three transport pathways (leaching, runoff, and plant uptake). While a single model is often preferred by practitioners, they generally exhibit substantial limitations that restrict their accurate or appropriate use. Current models are unable to model all the key parameters for the respective transport pathways. Therefore, a combination of models will be necessary to evaluate the three migration pathways and consider mass conservation.

The approach will vary depending on the circumstances and uncertainty surrounding the practices and pathways. If the estimated losses from all pathways combined is a small fraction of the mass of PFAS in applied residuals, then the models for each pathway can likely be run independently without consideration of losses from the other pathways. However, if losses from one or more of the pathways approach the mass of PFAS in applied residuals, the reduction in PFAS mass available for migration via the other pathways should be accounted for. For example, PFAS mass that runs off or transfers to plants will not leach to groundwater. Thus, the mass losses (or mass loss rates) from runoff and plant uptake models could be subtracted from the total mass used in the leaching model. A similar accounting for loss from leaching could be included when estimating losses via runoff or uptake by plants. It may be necessary to run the models iteratively to obtain a reasonable mass balance between the model inputs (mass in) and outputs (mass out) between the respective models. If there is significant uncertainty regarding the mass loss rates or mechanisms, then the losses from one pathway may be ignored when modeling another pathway(s).

Further, practitioners will need to account for the key PFAS parameters and other relevant modeling factors (e.g., residual application rate) and apply professional judgement based on the circumstances. This report recommends that PFAS be modeled as individual constituents given the wide range of physicochemical properties and toxicity of individual PFAS. Alternatively, some PFAS could be grouped

and modeled if they have similar model input properties and a linked regulatory standard or screening level.

The conclusions from the model reviews for each of the three migration pathways are summarized below.

5.1 Leaching

Thirty-one models were reviewed for the leaching pathway, and three models were identified as having the potential to model PFAS leaching (in alpha-numeric order):

- Hydrogeochem (4.0/5.0)
- Hydrus (1D, 2D, and 3D)
- SVENVIRO™.

None of the three models is able to model all of the key parameters that affect PFAS leaching from land-applied residuals. In particular, none of the models reviewed has the capability to model air-water interface partitioning. Because air-water partitioning (when present) is assumed to act as a mechanism that limits the mass of PFAS available to leach from land-applied residuals, the inability of these models to account for such partitioning is likely to result in the models overestimating the transport velocity and the concentration of PFAS in leachate. Such overestimates of PFAS concentrations in leachate may be acceptable depending on the purpose of the application of the models (e.g., developing conservative estimates of PFAS concentrations in leachate).

Other leaching models may also be suitable for PFAS modeling but were considered less applicable, as summarized in Section 2.3 and Table 2, because they were too complex to use, lacked key modeling capabilities, and/or exhibited documented limitations. However, they may be useful if their limitations are appropriately accounted for.

5.2 Surface Water

Thirty models were reviewed for the surface runoff pathway, of which one model was identified as having the potential to model PFAS leaching. PWC was identified as the most applicable to modeling PFAS at a field scale, where residuals are applied to a plot of land and PFAS concentrations in runoff need to be modeled. PWC was selected for its ability to model runoff as part of a water balance and its ability to characterize the interaction of soil with water (not just sheet flow as do other models), for its range of landcover scenarios, for the ability to enter site-specific weather data, and that applicable chemical-specific inputs that can be incorporated. In addition, transport-specific functions in the model handle complex nonlinear and nonequilibrium situations that may be exhibited by PFAS.

One of the limitations of PWC, and virtually all other models, is the ability to account for air-water interface partitioning (K_{ia}) and the surface tension effects. It is unclear exactly how K_{ia} and the surface tension effects of PFAS will affect surface water runoff from land-applied residuals. However, it is expected to be relatively minor because PFAS porewater concentrations in runoff from land-applied residuals are expected to be in the milligram per liter range or less, and the surface water runoff will effectively saturate

surrounding soils, reducing air-filled pore space in the soils, and thus reducing the effects of K_{ia} on runoff transport.

5.3 Plant Uptake

Twelve plant uptake models were identified and reviewed, of which only two were retained for further evaluation. While these two models appear to have the capability to model the uptake of PFAS by plants, they require plant-specific and PFAS-specific inputs that are not currently available for most plant species and PFAS. However, soil-to-plant TFs are available for a range of plant species and several individual PFAS. Until the required information is available for the two retained plant uptake models, soil-to-plant TFs from the literature can be used to estimate accumulation of PFAS in plants.

A compilation of literature-based soil-to-plant and soil solution-to-plant TFs for PFAS is presented in Table B-1 from the reviewed publications. A decreasing trend of soil-to-plant TFs with increasing carbon chain length appears to be present for both PFCA and PFSA. Solution-to-plant TFs show a similar trend for fruits, but the opposite trend for roots, with TFs increasing with increasing carbon chain length. Additionally, PFSA soil-to-plant TFs tend to be lower than PFCA soil-to-plant TFs for the same plant species and tissue type.

The TFs provided in the literature were mostly reported as the ratio of the concentration of PFAS in paired plant tissue and soil (or solution) samples and are not based on regression analysis of changes in PFAS concentration in plant tissue across a range of soil or solution concentrations. A more robust understanding and representation of PFAS accumulation in plants could be developed using regression analysis, assuming that suitable paired soil (or solution) and plant data are available. The compilation can also be used to identify additional data needs and research priorities to enhance the understanding of the factors that affect the accumulation of PFAS including different soil characteristics, different plant species and tissues, and varying PFAS characteristics (e.g., chain length and functional groups).

5.4 Research Needs

This review identified several areas of uncertainty regarding PFAS fate and transport modeling. The effect of that uncertainty on modeling of the three migration pathways could be better understood and the uncertainty reduced through additional research. Some of the areas where additional research would be most beneficial are listed below.

- Leaching to groundwater:
 - Assessment of PFAS desorption mechanisms
 - Assessment of PFAS sorption/desorption mechanisms such as air-water interfacial adsorption on transport
 - Assessment of PFAS effects on subsurface tension (pressure) and induced porewater flow.
- Runoff to surface water:

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- Assessment of PFAS desorption mechanisms residuals to runoff.
- Plant uptake:
 - Development of more robust TFs using regression analysis
 - Parameterization of mechanistic models, if deemed appropriate
 - Evaluation of particle deposition and plant uptake through leaves
 - Evaluation of the effect of soil characteristics, plant species, and tissue type on TFs.
- Application of models to actual residual land-application scenarios:
 - Determination of predictive ability of the models
 - Investigation of conservation of PFAS mass and relative importance of the three pathways.

Although additional research and model development may be necessary to accurately model PFAS transport, the existing models may be adequate depending on the application (e.g., developing conservative estimates of PFAS concentrations in runoff or leachate). The practicality and degree of improvement of the models will also need to be considered, as it may not be necessary to refine the models, particularly if they are used in a manner that accounts for their limitations.

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TABLES



Table 1
Relative Importance of Parameters in Modeling PFAS Fate and Transport
Review of Models for Evaluatin of PFAS in Residuals and Biosolids

Factor	Parameters of Relevance	Description	Availability of Data for Modeling	Relevance to Plant Uptake	Relevance to Surface Water Runoff	Relevance to Leaching	References for Data
Hydrophobic adsorption and desorption	K_{oc} - PFAS-specific f_{oc} - biosolids-specific	K_{oc} increases as-perfluoroalkyl chain length increases, with some exceptions	PFCAs - high PFAS - high PFAA precursors - low (available for some)	High; will affect PFAS concentrations in pore waters available for uptake	High	High	Anderson et al. 2019. Partitioning of poly-and perfluoroalkyl substances from soil to groundwater within aqueous film-forming foam source zones. <i>Journal of Contaminant Hydrology</i> . Vol. 220. Pages 59-65. Guello, J.L. and Higgins, C.P. 2013. Subsurface transport potential of perfluoroalkyl acids at aqueous film-forming foam (AFFF)-impacted sites. <i>Environmental Science & Technology</i> . Vol. 47 No. 9. Pages 4164-4171.
Soil to plant bioaccumulation	Bioaccumulation factor for different plant species and different PFAS	Many plants uptake PFAS from pore water; Some plants have exhibited preferential uptake of PFAS as chain length shortens, particularly fruits. Differences in bioaccumulation can vary by the part of the plant (i.e., leaves vs. roots).	Radish, tomato, celery, snap pea, strawberries, and lettuce for PFCAs and PFASAs	High	None	Not relevant	Blaine et al. 2014. Perfluoroalkyl acid distribution in various plant compartments of edible crops grown in biosolids-amended soils. <i>Environmental Science & Technology</i> . Vol. 48. Pages 7858-7865. Blaine, et al. 2014. Perfluoroalkyl acid uptake in lettuce (<i>Lactuca sativa</i>) and strawberry (<i>Fragaria ananassa</i>) irrigated with reclaimed water. <i>Environmental Science & Technology</i> . Vol. 48, No. 24. Pages 14361-14368. Blaine, et al. 2013. Uptake of perfluoroalkyl acids into edible crops via land applied biosolids: field and greenhouse studies. <i>Environmental Science & Technology</i> . Vol. 47 No. 24. Pages 14062-14069. Wen et al. 2016. The roles of protein and lipid in the accumulation and distribution of perfluorooctane sulfonate (PFOS) and perfluorooctanoate (PFOA) in plants grown in biosolids-amended soils. <i>Environmental Pollution</i> . Vol. 216. Pages 682-688.
PFAA generation from precursors	- Transformation rates of individual PFAS under different redox conditions - Soil ORP	PFAA precursors transform slowly to PFAAs; terminal conversion to PFAAs has only been observed under aerobic conditions, although partial transformation can occur under anaerobic conditions; transformation rates are significantly faster under aerobic conditions	Moderate; conversion of precursors to PFAAs can be modeled on the basis of redox conditions	Moderate/High - ongoing source term	Moderate/High - ongoing source term	Moderate/High, depending on types of PFAS in biosolids - ongoing source term	Mejia Avendano et al. 2016, Rhoads et al. 2008, Wang et al. 2005, Lee et al. 2010, Wang et al. 2011, Wang et al. 2009, Liu et al. 2010, Dasu et al. 2012, Harding-Marjanovic et al. 2015, Zhang et al. 2013, Zhang et al. 2016, Yi et al. 2018
Air water partitioning	K_{aw} - air water partitioning coefficient for different PFAS and possible sink	PFAS partition strongly at the air water interfaces common in unsaturated pore spaces	Moderate	Moderate - may reduce PFAS in pore water of unsaturated material	Moderate - dry biosolids may have lower contribution of PFAS to runoff	Moderate to High	Brusseau et al. 2019. Comprehensive retention model for PFAS transport in subsurface systems. <i>Water Research</i> . Vol. 148. Pages 41-50. Lyu et al. 2018. Adsorption of PFOA at the Air-Water Interface during Transport in Unsaturated Porous Media. <i>Environmental Science & Technology</i> . Vol 52. Pages. 7745-7753
Electrostatic adsorption	K_d - dependent on soil pH and composition and PFAS structure	K_d may be controlled more strongly by factors other than organic carbon partitioning depending on PFAS charge state (for cationic precursors in particular) and soil charge state, which is influenced in by pH and soil composition; cationic precursor relevance to biosolids is not well understood	K_d values are site-specific, and the literature values available are for compounds that cannot be measured in commercial laboratories. Data available for modeling is meager.	Moderate to Low - positively charged precursors will have lower uptake	Moderate to Low	Moderate to High	Xiao, et al. 2019. Sorption and desorption mechanisms of cationic and zwitterionic per-and polyfluoroalkyl substances in natural soils: Thermodynamics and hysteresis. <i>Environmental Science & Technology</i> . Barzen-Hanson et al. 2017. Sorption of fluorotelomer sulfonates, fluorotelomer sulfonamide betaines, and a fluorotelomer sulfonamide amine in national foam aqueous film-forming foam to soil. <i>Environmental Science & Technology</i> . Vol. 51. No. 21. Pages 12394-12404. Mejia-Avendaño et al. 2017. Assessment of the influence of soil characteristics and hydrocarbon fuel cointamination on the solvent extraction of perfluoroalkyl and polyfluoroalkyl substances. <i>Analytical Chemistry</i> . Vol. 89. No. 4. Pages 2539-2546.
Surface tension	Surface tension	PFAS can lower the surface and interfacial tension in pore water, increasing flow. Concentration-dependent	Limited to none at environmentally relevant concentrations.	Low	Low	Moderate to low	Lyu et al. 2018. Adsorption of PFOA at the air-water interface during transport in unsaturated porous media. <i>Environmental Science & Technology</i> . Vol 52. Pages 7745-7753. Guo et al. (in press). A mathematical model for the release, transport, and retention of per- and polyfluoroalkyl substances (PFAS) in the vadose zone. Manuscript accepted to <i>Water Resources Research</i> .
Volatilization	- H - loss term for individual compounds	Some volatile PFAS (e.g., fluorotelomer alcohols) may migrate out of biosolids and into soil gas or ambient air	H constants are available for volatile PFAS	Low	Low	Low	CONCAWE Environmental fate and effects of polyand perfluoroalkyl substances (PFAS). 2016
Fluorophilic interactions	K_d , soil- and PFAS-dependent	PFAS can self-assemble via fluorophilic interactions, particularly at interfaces; the effect of this factor will be embedded in K_d	K_d values are available, but are site-specific, for many PFAS	Low	Low	Low	
Solubility	Solubility	PFAS concentrations in residuals are expected to be well below the solubility limits	Solubility is available for many PFAS	Low	Low	Low	
PFAA decay	DT_{50} of individual compounds = 0 for PFAAs	PFAAs are not expected to break down under any environmentally relevant conditions	Not needed	None	None	None	

Notes:

DT_{50} = The time required for the concentration to decline to half the initial value (half-life).

f_{oc} = The tendency of PFAS to adsorb to soil organic matter

K_{ia} = Air water interface partitioning coefficient

K_d = Soil-water partitioning coefficient

K_{oc} = Organic carbon water equilibrium partitioning constant

ORP = Oxidation reduction potential

PFAA = Perfluoroalkyl acid

PFAS = Per- and polyfluoroalkyl substances

PFOA = Perfluoroalkyl carboxylate

PFSA = Perfluoroalkyl sulfonates

Table 2
 Review of Leaching Models for PFAS
 Review of Models for Evaluation of PFAS in Residuals and Biosolids

No.	Model	Public Domain	Costs	Analytical	Semi-analytical	Numerical	Finite Source	Steady State	Layering	Dual domain	1. Sorption/desorption (K_{oc}/K_d) [*]	2. Air-Water Interface Partitioning (K_{aw}) [*]	3. Electrostatic bonding (K_e)	4. Surfactant induced flow	5. Volatilization (K_v)	6. Degradation	7. Advection	8. Dispersion/diffusion	Advantages	Disadvantages	Retained (Y/#/N)	Links
1	CHEMFLO-2000	x	0			x		x	x						x	x	x		Models key PFAS parameters Free and peer-reviewed	Water flow model does not incorporate source term, so cannot simulate plant uptake at different depths. Sensitive to boundary conditions. Assumes partitioning is instantaneous and irreversible Significant discretization errors Primarily used in academia	N	http://www.epa.gov/water-research/chemflo-2000-interactive-software-simulating-water-and-chemical-movement-unsaturated
2	CMLS	x	0	x			x	x							x	x	x		Models key PFAS parameters Free and peer-reviewed	Chemical selection is based on a pre-populated list Does not have PFAS as optional chemicals Designed for agricultural uses (crop evapotranspiration and irrigation).	N	http://www.soilphysics.okstate.edu/software/cmls/index.html
3	FEFlow		\$\$- \$\$\$			x	x	x	x	x			?		x	x	x		User support and training 2D/3D graphics Ability to simulate multiple boundary conditions Can be coupled with user-created custom modules or modules purchased from DHI to expand capabilities	Costly, with long set-up times, and steep learning curve Transport modules not complete/under development (e.g., dual domain) Requires extensive modeling experience to use effectively European model Groundwater focused	N	https://www.mikepoweredbydhi.com/products/fflow
4	HYDRUS-1D (2D,3D)	x*	0-\$\$\$			x	x	x	x	x	x\$?	x	x	x	x	x		Inputs include most key PFAS parameters Code can be readily changed to model other key PFAS parameters Model is well maintained and adaptable, widely used/accepted 2D&3D & other add-ons (for fee). 1D is free	Packages necessary for complex sites or modeling of less critical PFAS parameters like electrostatic bonding need to be purchased at additional cost Adapting code requires advanced techniques & calibration	Y	http://www.pc-progress.com/en/Default.aspx?h3d-ver2
5	Hydrogeochem 4&5		\$\$\$			x	x	x	x	x	x		x	x	x	x	x		Inputs include most key PFAS parameters Widely reviewed/used	Site-specific, modeling of less critical PFAS parameters like electrostatic bonding would require add-on packages Cannot readily adapt code to the more critical PFAS parameters	Y	https://www.scientificsoftwaregroup.com/pages/product_info.php?products_id=44
6	PRZM / PWC	x	0	x	x		x	x					x	x	x	x	x		Designed for agricultural use and considers land application Widely used agrochemical industry Coupled with runoff, root zone, and plant uptake Developed and maintained by USEPA Free	Tipping bucket modeling, only considers downward advection Developed and tested for screening level assessments Unlikely to incorporate all important PFAS parameters	#	http://www.epa.gov/exposure-assessment-models/przm-version-index
7	SESOIL	x	0			x		x					x	x	x	x	x		Models key PFAS parameters including charge bonding Widely used/accepted Free	Not maintained	N	http://www.seview.com/
8	SEVIEW (SESOIL +AT123D)	x*	0-\$\$			x	x						x	x	x	x	x		Models key PFAS parameters including charge bonding Widely used/accepted Includes saturated zone fate and transport Includes runoff module	Source SESOIL code Limited heterogeneity allowed Weak runoff model Unlikely to incorporate all important PFAS parameters	#	http://www.seview.com/
9	Source Screening Module (SSM)	x*	0	x	x		x	x							x	x	x		Good for screening-level assessments (simple) Free	Does not appear to be peer reviewed Simplified model, not ideal for complicated sites	#	http://www.sspa.com/software/ssm
10	Stanmod	x	0	x	x		x	x						x	x	x	x		Vadose zone flow and solute transport code Well documented Free 1D, 2D, and 3D codes	Multiple computer codes included as part of STANMOD, and not all codes are able to include all features Homogenous, unidirectional systems only	#	https://www.pc-progress.com/en/Default.aspx?stanmod
11	SVENVIRO		\$\$\$			x	x?	x	x	x			?		x	x	x		CAD-based front end and automated solver. Accommodates multiple layers (including layers that pinch out). Borehole and soil survey data can be used to build model. Training offered. Cannot input user-defined isotherms for sorption processes	Costly Cannot readily adapt code to the more critical PFAS parameters	Y	https://soilvision.com/products/svoffice-ge/svchem-ge
12	VLEACH	x	0			x	x	x					x		x	x			Widely used/accepted Free	Focused on modeling volatile organic constituents Unlikely to be updated to model PFAS	N	http://www.epa.gov/water-research/vadose-zone-leaching-bleach
13	VS2DI	x	0			x	?	x	x						x	x			Models some key PFAS parameters 2D capabilities Free/public domain	Limited user input/control over the model Not focused on more complex chemical transport mechanisms Unlikely to be updated to model PFAS	#	https://www.usgs.gov/software/vs2di-version-13

Table 2
Review of Leaching Models for PFAS
Review of Models for Evaluation of PFAS in Residuals and Biosolids

No.	Model	Public Domain	Costs	Analytical	Semi-analytical	Numerical	Finite Source	Steady State	Layering	Dual domain	1. Sorption/desorption (K_{oc}/K_d)*	2. Air-Water Interface Partitioning (K_{aw})*	3. Electrostatic bonding (K_e)	4. Surfactant induced flow	5. Volatilization (K_v)	6. Degradation	7. Advection	8. Dispersion/diffusion	Advantages	Disadvantages	Retained (Y/#/N)	Links
14	VSAFT 2	x	0	x							?	x			x	x	x	Models some key PFAS parameters 2D capabilities Free/public domain	Appears to lack key capabilities for modeling PFAS. More academic. Documentation of model capabilities and model instructions are not clear. May also require validation/verification for some applications.	N	http://tian.hwr.arizona.edu/downloads	
15	TOUGH3		\$\$- \$\$\$		x	x	x	x	x	x		x	x	x	x	x	x	Models key PFAS parameters	Very complex, requiring high degree of expertise	#	https://tough.lbl.gov/software/tough-software/	
16	MODFLOW-USG + MT3DMS	x	0-\$\$\$		x	x	x	x	x	x		?	?	x	x	x		Models some key PFAS parameters Code can be readily changed to model other key PFAS parameters Model is well maintained and adaptable MODFLOW-USG + MT3DMS is publicly available for free	Complex, requiring moderate to high degree of expertise Adapting code requires advanced techniques & calibration User friendly GUI's and certain modules for fee from private vendors	#	https://www.usgs.gov/software/mt3d-usgs-groundwater-solute-transport-simulator-modflow	

Notes:

- 0 Free (public domain)
- \$ \$1 to \$700
- \$\$ \$701 to \$2,000
- \$\$\$ \$2,001+
- Y Yes, model limitations should be accounted for
- N No, model likely is not suitable for PFAS modeling
- # May be used under certain circumstances. Limitations should be accounted for.
- x model has capability
- x* model has capability at added cost (added modules may not be peer reviewed)

CAD = Computer-aided drafting

GUI = graphical user interface

PFAS = Per- and polyfluoroalkyl substances

List focused on models designed for assessing solute transport in the vadose zone

Bold, recommended for PFAS modeling. Add-on packages may be necessary and may not be suitable for complex sites. (See Descriptions)

Retained models are expected to be the most useful for modeling PFAS. However, other models can be used under certain conditions noting the limitations.

Table 3
Review of Surface Water Models for PFAS
Review of Models for Evaluation of PFAS in Residuals and Biosolids

Model	Public Domain (Y/N)	DT ₅₀	K _{oc}	Volatilization	K _{ai}	K _d	Land Cover Input	Advantages	Disadvantages	Retained (Y/N)	Links
3MRA	Y	Y	Y	Y	N	Y	Y	Has a land application unit (LAU) used to manage liquid, semi-solid, and solid wastes (biosolid applications).	Watershed scale model. Sheet flow is assumed across buffer subarea. Currently unable to enter site-specific and chemical-specific parameters (must be selected from a pre-defined list).	N	https://www.epa.gov/ceam/3mra
PWC	Y	Y	Y	Y	N	Y	Y	Can input site-specific and chemical-specific input parameters. The output reports the fraction of total constituent mass that was transported to the water body by runoff.	No land application residual scenario. But, can approximate by adjusting inputs and pre- &/or postprocessing data.	Y	https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/models-pesticide-risk-assessment
WEBMOD	Y	Y	Y	N	N	Y	Y	Simulates fluxes through watershed	Watershed scale model with complicated inputs Model response units (MRUs) discharge to one or more stream reservoirs that flow to the outlet of the watershed. No built in scenario to simulate land application Outputs are watershed-based, may be too broad for some sites	N	https://www.usgs.gov/software/water-energy-and-biogeochemical-model-webmod

Notes:

3MRA= Multimedia, Multi-pathway, Multi-receptor Exposure and Risk Assessment

DT₅₀= the time required for the concentration to decline to half of the initial value (half-life).

K_{ai}= air-water interface partitioning

K_d= electrostatic adsorption

K_{oc}= soil organic carbon-water partitioning coefficient

PWC= Pesticide in Water Calculator

WEBMOD= Water, Energy, and Biogeochemical Model

N = No

Y = Yes

Table 4
Review of Plant Uptake Models for PFAS
Review of Models for Evaluation of PFAS in Residuals and Biosolids

Model	Description	Rationale for Retention/Omission
Chiou et al. 2001	<p>Chiou et al. (2001) developed a mechanistic partitioning model that assumes passive root uptake is the main uptake mechanism for plant exposure to chemicals in soil. Dissolved organic chemicals are assumed to partition from water to root tissue and are then transported to other plant tissues through transpiration. The chemical concentration in pore water is estimated using a soil water partitioning coefficient. The chemical concentration in the transpiration stream is assumed to be the same as in pore water, and the concentration in the plant is estimated using a plant organic matter to water partitioning coefficient. This model features a dimensionless quasi-equilibrium factor defined as the ratio of a chemical in plant tissue to soil pore water (q_p). This factor can be calculated based on field observations or experimental studies. In generic modeling, the q_p can be assumed to be 1, representing the equilibrium condition assuming only passive root uptake from soil. For compounds with low solubility or a high octanol water partitioning coefficient (K_{ow}) (lipophilic), equilibrium may not be reached in leaves or tubers. As such, the assumption regarding reaching equilibrium is conservative, and the q_p for such compounds may be less than 1. The key input parameters for this model are K_{ow}, the weighted average plant lipid fraction, water and carbohydrate content, and the fraction of soil organic carbon.</p>	<p>Because this model was developed for non-ionic organic compounds, and PFAS are positively and negatively charged at typical environmental pH and tend to partition to proteins rather than lipids, this model is unlikely to be predictive of PFAS partitioning behavior in plants.</p>
Hung and Mackay 1997	<p>Hung and Mackay developed a comprehensive dynamic fugacity-based model to estimate the concentration of organic chemicals in herbaceous agricultural plants. The model divides plants into three compartments: root, stem, and leaf. The processes included in the model are root uptake, chemical transport via xylem and phloem, air-leaf exchange, growth dilution, and metabolism. A steady-state mass balance model using partition coefficients is used for each compartment. The partitioning coefficients could be either measured or calculated using correlations with physical chemical properties. This model requires several plant- and chemical-specific properties including compartment volumes, xylem flow rate, phloem flow rate, diffusive and bulk flow rates from soil to root, air-leaf exchange rates, partitioning coefficients between various compartments, growth, and metabolism half-lives.</p>	<p>This model is not practical for application to PFAS because it is data-intensive, including requiring PFAS-specific partition coefficients. Furthermore, fugacity-based models are more suitable for modelling the behavior of neutral organic compounds in the environment.</p>
Ryan et al. 1988	<p>Ryan et al. (1988) developed a partitioning model that estimates the equilibrium soil-to-root and soil-to-stem concentration factors. This model was developed based on experimental data from Briggs et al. (1982, 1983). Those data report a correlation between K_{ow} and the concentration of compounds in roots and stems. The experimental study investigated the uptake of two non-ionized compounds (i.e., o-methylcarbamoyloximes and substituted phenylureas) by barley roots and shoots. Passive root uptake was the dominant transport mechanism for these two chemicals. Ryan et al. (1988) incorporated the soil adsorption potential of hydrophobic chemicals into the uptake model and assumed that soil adsorption potential can be estimated using an organic carbon-water partitioning coefficient (K_{oc}). The model applies a correction factor to account for lower bioavailability of chemicals in soil compared to the aqueous solution used in the plant uptake study. The input parameters for this model are K_{ow} and K_{oc}, and soil parameters including soil bulk density, water filled soil porosity, and fraction organic carbon.</p>	<p>This is a semi-mechanistic model relies on experimental data on two chemicals with transport behavior that differs from PFAS and only one plant species. As such, this model unlikely to be predictive of uptake of PFAS by most plant species.</p>
Topp et al. 1986	<p>Topp et al. (1986) developed a regression model based on experimental studies on plant uptake of organic chemicals from soil and air (after volatilization). They studied the uptake of 16 radioactively labelled neutral and ionic organic chemicals by barley and cress seedlings in a 7-day experiment. The chemicals included benzene, atrazine, pentachlorophenol, a selection of chlorobenzenes, and DDT. Some correlation between soil pore water concentration and plant concentration, foliar uptake, and air concentration was noted. However, the strongest correlation was observed between molecular weight of a compound and overall plant uptake. The molecular weight of tested compounds ranged from 75 to 600 grams per mole.</p>	<p>The applicability of this model is limited because a correlation between the concentration of chemicals in soils and plants could not be established as only the radioactively labelled carbon concentration was measured. A second limitation is that the model may not be valid for plants with lipid concentrations different than that of barley.</p>
Travis and Arms 1988	<p>Travis and Arms (1988) reviewed more than 20 different studies and compiled transfer factors, or reported concentrations in plants and corresponding soil, for 29 organo-chlorine chemicals. They developed a regression model to predict the soil-to-plant transfer factors for aboveground parts as a function of $\log K_{ow}$ on a dry mass basis. This model is easy to use and is based on empirical data for different chemicals and plant types.</p>	<p>The model has been calibrated for chemicals with $\log K_{ow}$ ranging from 1 to 10. Because this model was developed for non-ionic organic compounds and relies on K_{ow} to predict uptake, it is unlikely to be predictive of PFAS partitioning behavior in plants.</p>
USEPA MMSOILS Model	<p>The multimedia contaminant fate, transport, and exposure model (MMSOILS) was developed by the USEPA and released in 1997 to estimate potential human health risks associated with exposure to chemicals in the environment. MMSOILS includes exposure from consumption of terrestrial plants and root vegetables grown on contaminated soil. The accumulation of chemicals in aboveground plants is modelled through two mechanisms: atmospheric deposition onto the aerial parts of plants and root uptake. MMSOILS uses the deposition equation by Moghissi et al. (1980) to estimate plant concentrations from atmospheric deposition. Uptake from soil is estimated using soil to plant transfer factors developed by Baes (1982) for metals and by Travis and Arms (1988) for organic chemicals. The concentration in aboveground plant tissues is estimated as the sum of concentrations due to deposition and uptake from soil.</p> <p>The concentration in root crops is estimated using a root concentration factor (RCF), chemical concentration in soil, and soil moisture. Briggs et al. (1982) developed an empirical equation as a function of $\log K_{ow}$ based on uptake of chemicals by barley roots and compared the results with published</p>	<p>MMSOILS could be used for modeling uptake of PFAS if PFAS-specific soils-to-plant transfer factors are available. Air-to-plant deposition is likely less relevant for PFAAs, as these compounds are not volatile at environmentally relevant pH.</p>

Table 4
Review of Plant Uptake Models for PFAS
Review of Models for Evaluation of PFAS in Residuals and Biosolids

Model	Description	Rationale for Retention/Omission
Trapp and Co-Workers (since 1995)	<p>data on chemical uptake by roots of corn, tomatoes, soybean, and rice. The correlation matches the data for a wide variety of chemicals and plants relatively well.</p> <p>Trapp and co-workers (Trapp 2015, 2007; Trapp and Matthies 1995) have developed a comprehensive mechanistic plant uptake model (known as the standard model) based on physical fluxes and partitioning processes among various plant compartments including roots, stems, and leaves. Trapp and Matthies (1995) developed a one-compartment model for leafy vegetables (i.e., aboveground plants). This model considers several uptake and loss processes including passive root uptake, translocation from roots to shoots, air-leaf exchange, metabolism, and growth. This model has been used by the European Union System for the Evaluation of New and Existing Substances (EUSES) for screening potential risks associated with plant uptake (EU 2003). This model is only applicable to neutral (non-ionized) compounds. Input parameters include plant-specific, chemical-specific, and soil parameters. The plant-specific parameters have default values in the EUSES model. The chemical-specific parameters are K_{ow} and Henry's law constant. Soil parameters are soil bulk density, water-filled soil porosity, and fraction of organic carbon.</p> <p>The application of the standard model for neutral organic compounds was further investigated in two subsequent studies by Trapp (2007 and 2015). Trapp (2007) developed an eight-compartment fruit tree model to predict the concentration of neutral organic chemicals from soil and air into fruits. Trapp (2015) calibrated the standard model for radish with plant- and site-specific data for the uptake of chlorinated organic compounds from soil to radish.</p> <p>Trapp (2004) reviewed models for plant uptake of electrolytes. For electrolytes, the ion concentration at the membranes follow the Nernst-Planck law while, for neutral compounds, the diffusion across membrane follows Fick's First Law. In a subsequent study, Trapp (2009) used models to examine the uptake of neutral and ionized organic compounds and compared model predictions to experimental results. Several additional processes, including dissociation, ion trap effects, and electrical attraction and repulsion, were noted for bioaccumulation of ionized chemicals in plants, and the effects of pK_a and pH were found to be more important than lipophilicity.</p> <p>Trapp has developed dynamic and steady-state soil-plant uptake models for monovalent organic chemicals, such as pesticides and pharmaceuticals, to understand the distribution of ionizable compounds in the soil-root-leaf system (Trapp 2017). These models follow the principles of the standard model developed for neutral organics and have been supplemented with a cell model for the calculation of partitioning coefficients of ionizable compounds. The steady-state model assumes transport of chemicals via xylem from soil to roots to leaves; and via phloem from leaves to roots. The steady-state model has been coupled with a cell model in which the partitioning coefficients among root-to-water, xylem-to-water, phloem-to-xylem, and vacuole-to-water are calculated after a defined period of time. It uses water, protein, and lipid content of various plant tissues including cytoplasm, xylem, phloem, and vacuole. Steady-state model input parameters include K_{ow} for both neutral and ionic species, air-water partitioning coefficient (K_{aw}), partitioning coefficient for adsorption to protein, pK_a, ion strength of soil, and data on plant morphology among other factors. As noted in the disclaimer of the model "<i>The plant uptake models for ionisable compounds, such as pesticides and pharmaceuticals, contain many parameters that are rarely known in detail and variable in time. The models therefore usually do not predict exact concentrations.</i>"</p> <p>Very recently, Gredelj et al. (2020) modeled the uptake of PFAA in soil into plants using a semi-empirical model. The purpose was to understand PFAA partitioning behavior in plants and identifying the plant-specific factors that control and affect uptake of PFAA. Gredelj et al. (2020) calibrated the Trapp and co-worker standard model (Trapp 2015, 2007; Trapp and Matthies 1995) using experimental data from Gredelj et al. (2019) on plant uptake of nine PFAA from soil into red chicory. The model was modified to include the dry weight-based RCFs available from other experimental studies. A new factor, referred to as retardation factor (R), was introduced in the model. R is defined as the concentration ratio between the xylem sap and soil pore water and is equivalent to the ratio of root permeability for a chemical to that of water. For PFAA, R is expected to be less than 1, as the uptake of PFAA into roots is slower than the uptake of water into roots. R is a function of the transpiration stream concentration factor (TSCF) and root to xylem partitioning coefficient (K_{rx}). The PFAA-specific model input parameters were obtained from Gredelj et al. (2019). The model overpredicted concentrations in red chicory leaves but were similar to measured concentrations in red chicory heads for several PFAA. In general, model performance was shown to be better for PFCAAs than PFSAs and better at lower than higher soil concentrations (i.e., 100 rather than 200 nanograms per gram (ng/g)).</p>	<p>Using PFAA R values derived for red chicory and parameters such as K_d, growth time and water content from other studies, Gredelj et al. (2020) predicted PFAAs concentrations in roots, shoots, and fruits of tomato, celery, pea, and radish. The predicted PFAA concentrations in shoots were within one order of magnitude of measured values with better estimates for short-chain than long-chain PFAAs and for tomato and peas than for radish and celery. While such detailed mechanistic plant uptake models have the capability to estimate PFAA concentration in various parts of plants, the need for site-specific inputs for some key parameters, such as K_d, growth time, and RCF, is crucial to accurate model performance making such mechanistic models impractical for screening purposes.</p>
Plant Uptake Model Based on Irrigation Water	<p>The Canadian Standard Association developed N288.1 (CSA 2014) to estimate plant uptake of inorganic compounds from impacted spray irrigation water. The model assumes that irrigation water wets leaves as well as soil. Chemicals in irrigation water on leaves are assumed to be taken up directly by leaves, and chemicals in soil are assumed to be taken up by roots. The two processes are modeled separately and the resulting concentrations are summed to estimate the overall concentration in plants. The input parameters include leaf area index, volume of water retained per unit of ground surface area, frequency of irrigation, a translocation factor from foliage to consumable parts, harvest index, effective removal constant from vegetation surfaces, effective duration of the deposition, and yield of consumable plant product per unit area. Literature-based soil-to-plant transfer factors are used to predict the concentrations of chemicals in plants from impacted soil. The model conservatively assumes that losses due to erosion, leaching, and crop removal are negligible, although leaching could be an important loss process for short-chain PFAA.</p>	<p>Because this is a model based on empirical data for inorganics, if parallel empirical data were available for PFAS, the model is likely to be applicable to PFAS. However, currently the necessary empirical data are not available for most PFAS and models such as CSA N288.1 have not been applied to PFAS.</p>

For full references associated with the citations in this table, please refer to the References section in the main report.

APPENDIX A

Model Screening



Table A-1
Screening of Leaching Models for PFAS
Review of Models for Evaluation of PFAS in Residuals and Biosolids

No.	Model	Public Domain (Y/N)	Costs (0,\$,\$\$,,\$\$,\$\$\$)	Supported/Maintained (Y/N)	Last Update	Peer Reviewed (Y/N)	Summary	Retained (Y/N)	Basis for Rejecting
Analytical Mixing Models									
1	New Jersey Solution	Y	0	Y	?	Y	Agency-dependent (USEPA established basic protocols)	N	Infinite source, no retardation
2	USEPA Soil to Groundwater Pathway Screening Calculations	Y	0	n/a	n/a	Y	Simple analytical equilibrium/mixing model to screen constituents or sites	N	Infinite source, no retardation
3	Complete Mixing Model (Summer's Model)	Y	0	n/a	n/a	Y		N	Infinite source, no retardation
Semi-Numerical and Numerical Models									
4	2D & 3DFATMIC	Y	0	N	1997 (Version 1)	Y	2D and 3D model simulates subsurface flow, fate and transport of constituents that are undergoing chemical or biological transformations. The model is applicable to transient conditions in both saturated and unsaturated zones.	N	Obsolete - software is not maintained/supported Rarely used
5	3DFEMWATER & 3DLEWASTE	Y	0	N	1993 (Version 1)	Y	3D Finite element model of flow and transport through saturated and unsaturated media (3DFEMWATER) and 3D Lagrangian-Eulerian Finite Element Model of Waste transport through saturated and unsaturated media (3DLEWASTE) are related models that can be used to model groundwater flow and constituent transport in 3D under variably saturated conditions.	N	Obsolete - software is not maintained/supported Noted bugs, rarely used Only code is provided
6	3MRA	Y	0	N?	2003 (still on Version 1)	Y	Multimedia, Multi-pathway, Multi-receptor Exposure and Risk Assessment (3MRA). Assessment tool that is national in scale and site-based. In other words, risks are assessed at individual sites across the U.S. where waste management units may be located.	N	Designed for large scale screening risk assessments. Only 46 constituents in 3MRA database & does not include PFAS
7	BIOF&T	N	\$\$	Y	1997	?	BIOF&T models biodegradation and 2D water flow and transport in saturated and unsaturated zones.	N	Does not include PFAS in any of the databases.
8	CHEMFLO-2000	Y	0	Y	2003 Version 2000	Y	CHEMFLO-2000 was designed as an interactive, educational tool to numerically simulate 1D water movement and chemical fate and transport in vadose zones.	Y	N/A
9	CMLS	Y	0	Y	2005 5th update)	Y	Chemical Movement in Layered Soils (CMLS) model was developed as a management tool for agricultural organic chemicals. CMLS can be used to estimate the movement of chemicals in soils in response to downward movement of water. The model also estimates the degradation of the chemical and the amount remaining in the soil profile.	Y	N/A
10	FEFlow	N	\$\$-\$\$\$	Y	2019 Version 7.2	Y	FEFlow numerically models water flow and constituent transport using finite element methods. The software is capable of modeling local to regional (i.e., watershed) areas and uses a GUI. Add-on modules (either user-defined or available for purchase) can extend the capabilities of the program.	Y	N/A
11	HYDRUS1D	Y	0	Y	2018 Version 4	Y	Hydrus1D numerically models 1D water flow and constituent and heat transport in saturated and unsaturated conditions using finite element methods. The software uses a GUI.	Y	N/A
12	HYDRUS2D,3D,...	Y/N	\$\$-\$\$\$	Y	2018 Version 3	Y	Hydrus2D and Hydrus3D model 2D and 3D water flow and constituent and heat transport in saturated and unsaturated conditions using finite element methods. The software uses a GUI. Add-on modules(available for an additional fee) can extend the capabilities of the program.	Y	N/A
13	Hydrogeochem	N	\$\$-\$\$\$	Y	2018	Y	HYDROGEOCHEM is a coupled hydrologic transport and geochemical reaction model for transient or steady-state transport of constituents in saturated and unsaturated media.	Y	N/A
14	MODFLOW-USG + MT3DMS	Y	0	Y	2019 Version 1	Y	MODFLOW-USG + MT3DMS simulates 3D water flow and constituent transport under saturated and unsaturated conditions using control volume finite difference methods. This version of MODFLOW incorporates a flexible grid design and the groundwater flow process and connected linear network modules from MODFLOW-2000.	Y	N/A

Table A-1
Screening of Leaching Models for PFAS
Review of Models for Evaluation of PFAS in Residuals and Biosolids

No.	Model	Public Domain (Y/N)	Costs (0,\$,\$\$,\$\$\$\$)	Supported/Maintained (Y/N)	Last Update	Peer Reviewed (Y/N)	Summary	Retained (Y/N)	Basis for Rejecting
15	MULTIMED	Y	0	N?	1996 Version 2 Beta	Y	MULTIMEDIA exposure assessment model; for exposure assessment simulates the movement of constituents leaching from a waste disposal facility. The model consists of a number of modules that predict concentrations at a receptor due to transport in the subsurface, surface air, or air.	N	DOS only and not supported/maintained
16	ParFlow	Y	0	Y	2017 Version 3	Y	ParFlow was designed for water cycle research and simulates surface and subsurface 3D flow under saturated and unsaturated conditions using a large grid format to simulate large areas (i.e., watershed scale or larger).	N	Chemical fate and transport are not modeled
17	Pollute	N	\$\$	Y	? Version 7	?	Pollute was intended for landfill design and remediation, and used a 1.5-dimensional solution to simulate advective-dispersive constituent transport in the subsurface under variably saturated conditions.	N	Designed for lined landfill usage
18	PRZM / PWC	Y	0	Y	2016 Version 5	Y	Pesticide Root Zone Model (Version 5), part of Pesticide in Water Calculator (PWC) model, was designed for modeling pesticide and nitrogen transport after agricultural application. PRZM/PWC is a 1D finite-difference model with a GUI.	Y	N/A
19	RITZ	Y	0	N	1988 2.12	N?	Regulatory and Investigative Treatment Zone (RITZ) model is a steady-state analytical model used to simulate the transport and fate of chemicals mixed with oily wastes (sludge) and disposed of by land treatment.	N	Disk operating system (DOS) interface only and not supported/maintained
20	SESOIL	Y	0-\$	Y	2003	Y	SEASONAL SOIL (SESOIL) compartment model is a 1D vertical transport simulation for vadose zone (unsaturated) models. SESOIL includes a runoff module.	Y	N/A
21	SEVIEW (SESOIL +AT123D)	N	\$\$	Y	2017? Version 7	Y	SEVIEW couples SESOIL with AT123D and a GUI to model constituent transport under 1D groundwater flow with or without biodegradation. SEVIEW can incorporate multiple source areas.	Y	N/A
22	Source Screening Module (SSM)	Y*	0	Y	2018	?	SSM was developed as a screening tool to classify sites based on risk to groundwater systems. SSM is a simple, quasi 2D, Excel-based Visual Basic for Applications (VBA) leaching model that simulates constituent transport from a source area, through the vadose zone, and through the saturated zone to a receptor well.	Y	N/A
23	STANMOD (USDA)	Y	0	N?	2003 Version 2	Y	STUDIO of ANALYTICAL MODELS (STANMOD) was designed to incorporate several pre-existing solute transport models into one software program. STANMOD is a 1D analytical transport model for evaluating constituent transport with convection-dispersion equations and uses a similar GUI as HYDRUS1D and HYDRUS2D.	Y	N/A
24	STOMP	N	\$\$-\$	Y	?	Y	Subsurface Transport Over Multiple Phases (STOMP) is a sequential numerical program designed for the general simulation of 3D multiphase water flow and constituent transport using partial-differential equations and integrated-volume finite-difference methods. Certain versions of STOMP are publicly available, while others are restricted for research use only.	N	Focused on research regarding variable phase constituents/fluids
25	SUTRA (USGS)	Y	0	Y?	2019 Version 3	N?	Saturated-Unsaturated TRANSPORT (SUTRA) model was designed to simulate 1D, 2D, and 3D variable-density water flow, solute transport, and heat flow using finite element and finite difference methods. Simulations can be run under transient or steady-state conditions.	N	Focused on variable density fluids & heat
26	SVENVIRO (SVFLUX with SVCHEM)	N	\$\$\$	Y	2018	Y	SVENVIRO™ was designed to model groundwater seepage in unsaturated or saturated soils and rock. It is offered as a comprehensive 1D, 2D, and 3D finite-element program for calculating steady-state and transient-state groundwater flow. The model combines a CAD-based 2D and 3D GUI with the groundwater modeling abilities of the Finite element and Heat Mass Transfer (FEHM) solver developed by Los Alamos National Laboratory (LANL). Regional flow models, including many pumping wells with complex geometry, can be modeled.	Y	N/A
27	TOUGH3	N	\$\$\$	Y	2018	Y	TOUGH ("Transport Of Unsaturated Groundwater and Heat") suite of software codes are multi-dimensional numerical models for simulating the coupled transport of water, vapor, non-condensable gas, solute, and heat in porous and fractured media. 3D multiphase/unsaturated flow & transport.	Y	N/A

Table A-2
 Screening of Surface Water Models for PFAS
 Review of Models for Evaluation of PFAS in Residuals and Biosolids

Model	Public Domain (Y/N)	Supported/Maintained (Y/N)	Peer Reviewed (Y/N)	Summary	Retained (Y/N)	Basis for Rejecting
MULTIMED 2.0 Beta	Y	N (last update 1996)	Y	MULTIMED is a multimedia exposure assessment model that simulates the movement of contaminants leaching from a waste disposal facility.	N	Leaching from disposal facility. Cannot control key aspects of surface water module. Only runs on DOS or Fortran. Not maintained/supported.
MULTIMED (Daughter Process)	Y	N (last update 1996)	Y	The MULTIMED model has been modified (MULTIMDP) to simulate the transport and fate of first- and second-generation transformation (daughter) products that migrate from a waste source through the unsaturated and saturated zones to a downgradient receptor well.	N	Leaching from disposal facility. Cannot control surface water module. Can only open through DOS or Fortran. Not readily accessible with current operating system.
3MRA	Y	Y	Y	The Multimedia, Multi-pathway, Multi-receptor Exposure and Risk Assessment (3MRA) technology provides the ability to conduct screening-level risk-based assessment of potential human and ecological health risks resulting from long-term (chronic) exposure to Hazardous Waste Identification Rule (HWIR) chemicals released from land-based waste management units (WMUs) containing currently listed waste streams. The 3MRA system consists of a series of components within a system framework. The new modeling system, dubbed 3MRA technology, is envisioned as the foundation for eventually integrating other regulatory support decision tool needs anticipated in the future.	Y	N/A
MMSOILS	Y	N (last update 1996)	Y	The Multimedia Contaminant Fate, Transport, and Exposure Model (MMSOILS) estimates the human exposure and health risk associated with releases of contamination from hazardous waste sites. The methodology consists of a multimedia model that addresses the transport of a chemical in groundwater, surface water, soil erosion, the atmosphere, and accumulation in the food chain.	N	Only works with DOS operating system.
EXAMS	Y	Y	Y (3MRA)	The Exposure Analysis Modeling System (EXAMS) is an interactive software application for formulating aquatic ecosystem models and rapidly evaluating the fate, transport, and exposure concentrations of synthetic organic chemicals including pesticides, industrial materials, and leachates from disposal sites.	N	EXAMS is run in conjunction with other models. EXAMS is already being considered within the framework of 3MRA.
Express	Y	Y	Y	EXPRESS (EXAMS - PRZM Exposure Simulation Shell) is designed to facilitate a rapid and consistent assessment of aquatic pesticide exposure on a variety of crops. EXPRESS is a joint project of the USEPA Office of Pesticide Programs' Environmental Fate and Effects Division (OPP/EFED) and the USEPA Office of Research and Development (ORD).	N	Model is for drinking water and aquatic exposure assessments. Doesn't account for concentrations in runoff.
PRZM3	Y	Y	Y	PRZM3 is the most recent version of a modeling system that links two subordinate models (PRZM and VADOFT) to predict pesticide transport and transformation down through the crop root and unsaturated zone	N	Accounts for crop root zone and unsaturated zone. Not runoff-based.
SWMM	Y	Y	Y	USEPA's Stormwater Management Model (SWMM) is used throughout the world for planning, analysis, and design related to stormwater runoff, combined and sanitary sewers, and other drainage systems. It can be used to evaluate gray infrastructure stormwater control strategies, such as pipes and storm drains, and is a useful tool for creating cost-effective green/gray hybrid stormwater control solutions. SWMM was developed to help support local, state, and national stormwater management objectives to reduce runoff through infiltration and retention, and help to reduce discharges that cause impairment of our Nation's waterbodies.	N	SWMM was designed for the assessment of urban runoff. According to open source SWMM dialogue, it is not intended for rural watersheds absent abundant long-term calibration data for that specific site. Assumes sheet flow over a pervious catchment area, and calculates the infiltration based on the full area of the catchment. Generally runoff forms rivulets/puddles and infiltration is considerably less.
PWC	Y	Y	Y	The Pesticide in Water Calculator (PWC) is an updated version of the tool previously known as the Surface Water Concentration Calculator (SWCC). The tool's name was changed to better reflect that PWC can now simulate both surface water and groundwater. In addition, PWC has an improved volatilization routine and more batch run capabilities. PWC version 1.52 is the latest version approved for regulatory use. It is composed of a graphical user interface, a field model (PRZM version 5.02), and a water body model: (VWMM version 1.02).	Y	N/A
SWAT	Y	Y	Y	The Soil & Water Assessment Tool is a small watershed to river basin-scale model used to simulate the quality and quantity of surface and groundwater and predict the environmental impact of land use, land management practices, and climate change. SWAT is widely used in assessing soil erosion prevention and control, non-point source pollution control, and regional management in watersheds.	N	This is a model for watersheds and allows inputs for point sources. It does not appear that residual application to farm fields or forests could be modeled. This appears to be a larger-scale model with many inputs on a watershed basis (rather than small field or plot).

Table A-2
 Screening of Surface Water Models for PFAS
 Review of Models for Evaluation of PFAS in Residuals and Biosolids

Model	Public Domain (Y/N)	Supported/Maintained (Y/N)	Peer Reviewed (Y/N)	Summary	Retained (Y/N)	Basis for Rejecting
APEX	Y	Y	Y	APEX has components for routing water, sediment, nutrients, and pesticides across complex landscapes and channel systems to the watershed outlet as well as groundwater and reservoir components. A watershed can be subdivided as much as necessary to ensure that each subarea is relatively homogeneous in terms of soil, land use, management, and weather. APEX was constructed to evaluate various land management strategies considering sustainability, erosion (wind, sheet, and channel), economics, water supply and quality, soil quality, plant competition, weather, and pests. The routing of water, sediment, nutrient, and pesticide capabilities are some of the most comprehensive available in current landscape-scale models and can be simulated between subareas and channel systems within the model	N	While this model may be able to account for PFAS losses in runoff, the scale is likely to large as this is a watershed-scale model and is also likely more complex than necessary for application on a smaller scale.
WINSRFR 5.1	Y	Y	Y	WinSRFR is a hydraulic analysis tool for surface irrigation systems. The simulator predicts the surface and subsurface flow of water as a function of system geometry, infiltration, hydraulic resistance, and inflow management. The software also integrates evaluation, operational analysis, and design functionalities for surface irrigation systems. The simulator predicts the surface and subsurface flow of water as a function of system geometry, infiltration, hydraulic resistance, and inflow management.	N	This model is for irrigation management and does not appear to be readily applicable to estimating concentration of chemicals in runoff.
AGWA	Y	Y	Y	The Automated Geospatial Watershed Assessment (AGWA) tool is a GIS-based hydrologic modeling tool that uses commonly available GIS data layers to fully parameterize, execute, and spatially visualize results for the RHEM, KINEROS2, KINEROS-OPUS, SWAT2000, and SWAT2005 watershed runoff and erosion models.	N	This is a visualization tool for other models.
KINEROS 2 RUNOFF MODEL	Y	Y	Y	The kinematic runoff and erosion model KINEROS is an event-oriented, physically based model describing the processes of interception, infiltration, surface runoff, and erosion from small agricultural and urban watersheds. The watershed is represented by a cascade of planes and channels; the partial differential equations describing overland flow, channel flow, erosion, and sediment transport are solved by finite difference techniques. The spatial variation of rainfall, infiltration, runoff, and erosion parameters can be accommodated.	N	Does not model chemical runoff, but, could be used to accurately estimate water runoff.
RHEM	Y	Y	Y	RHEM is designed to provide sound, science-based technology to model and predict runoff and erosion rates on rangelands and to assist in assessing rangeland conservation practice effects. RHEM is a newly conceptualized, process-based erosion prediction tool specific for rangeland application, based on fundamentals of infiltration, hydrology, plant science, hydraulics and erosion mechanics.	N	RHEM is specifically for rangeland and doesn't have a component for modeling chemical inputs.
HIRO2	Y	N	N	HIRO2 (Hortonian Infiltration and Run-Off/On) is a spatially distributed rainfall-runoff model for event-based studies of space-time watershed processes. A grid-based routing hierarchy was defined over the watershed using the D-infinity contributing area algorithm. Computation of ponding time was included to handle variable run-on and rainfall intensity. The Green-Ampt model was adopted to calculate surface infiltration, and the kinematic wave model was used to route Hortonian runoff and channel flow. The model can handle input rainfall, soil parameters, surface roughness, and other properties that vary in space and time.	N	This is a hydrology-based model and does not appear to have the ability to accept chemical inputs associated with land application data.
SMALL WATERSHED HYDROLOGY (WINTR-55)	Y	Y	Y	WinTR-55 is a single-event rainfall-runoff small watershed hydrologic model. The model generates hydrographs from both urban and agricultural areas and at selected points along the stream system. Hydrographs are routed downstream through channels and/or reservoirs. Multiple sub-areas can be modeled within the watershed.	N	This is a hydrology-based model with hydrographs as outputs.
HSPF	Y	Y	Y	Hydrological Simulation Program - FORTRAN (HSPF) is a comprehensive package for simulation of watershed hydrology and water quality for both conventional and toxic organic pollutants. HSPF incorporates watershed-scale ARM and NPS models into a basin-scale analysis framework that includes fate and transport in one-dimensional stream channels. It is the only comprehensive model of watershed hydrology and water quality that allows the integrated simulation of land and soil contaminant runoff processes with in-stream hydraulic and sediment-chemical interactions. The result of this simulation is a time history of the runoff flow rate, sediment load, and nutrient and pesticide concentrations, along with a time history of water quantity and quality at any point in a watershed. HSPF simulates three sediment types (sand, silt, and clay) in addition to a single organic chemical and transformation products of that chemical.	N	Maybe as part of BASINS but BASINS is a complicated, watershed-based, GIS model. It would require a lot of inputs in order to obtain values for runoff and not certain we need a history of runoff rate and history of chemical concentrations at any point in a watershed as outputs.

Table A-2
 Screening of Surface Water Models for PFAS
 Review of Models for Evaluation of PFAS in Residuals and Biosolids

Model	Public Domain (Y/N)	Supported/Maintained (Y/N)	Peer Reviewed (Y/N)	Summary	Retained (Y/N)	Basis for Rejecting
BASINS	Y	Y	Y	Better Assessment Science Integrating Point and Nonpoint Sources (BASINS) is a multipurpose environmental analysis system designed to help regional, state, and local agencies perform watershed- and water quality-based studies.	N	Complicated, GIS and watershed-based model.
FESWMS-2DH	Y	Y	Y	FESWMS-2DH is a modular set of computer programs that simulates two-dimensional, depth-integrated, surface-water flows. FESWMS-2DH consists of an input data preparation program (DINMOD(1)), flow model (FLOMOD(1)), simulation output analysis program (ANOMOD(1)), and graphics conversion program (HPLOT(1)). The programs have been developed to analyze flow at bridge crossings where complicated hydraulic conditions exist, although they may be applied to many types of steady or unsteady flow problems. Shallow rivers, flood plains, estuaries, and coastal seas are examples of surface-water bodies in which flows may be essentially two-dimensional in the horizontal plane.	N	FESWMS-2DH was developed to analyze flow at bridge crossings where complicated hydraulic conditions exist. This model only simulates water flows and does not allow for water quality parameters inputs.
GSFLOW	Y	Y	Y	GSFLOW is a coupled Groundwater and Surface-water FLOW model based on the integration of the USGS Precipitation-Runoff Modeling System (PRMS-V) and the USGS Modular Groundwater Flow Model (MODFLOW-2005 and MODFLOW-NWT). GSFLOW was developed to simulate coupled groundwater/surface-water flow in one or more watersheds by simultaneously simulating flow across the land surface, within subsurface saturated and unsaturated materials, and within streams and lakes. Climate data consisting of measured or estimated precipitation, air temperature, and solar radiation, as well as groundwater stresses (such as withdrawals) and boundary conditions, are the driving factors for a GSFLOW simulation.	N	GSFlow was developed to simulate coupled groundwater/surface-water flow and does not allow for water quality parameter inputs.
LOADEST	Y	Y	Y	LOAD ESTimator (LOADEST) is a FORTRAN program for estimating constituent loads in streams and rivers. Given a time series of streamflow, additional data variables, and constituent concentration, LOADEST assists the user in developing a regression model for the estimation of constituent load (calibration). Explanatory variables within the regression model include various functions of streamflow, decimal time, and additional user-specified data variables. The formulated regression model is then used to estimate loads over a user-specified time interval (estimation). Mean load estimates, standard errors, and 95 percent confidence intervals are developed monthly and (or) seasonally.	N	LOADEST estimates mass of suspended sediment or chemical constituent entering a lake or estuary from a river or stream but does not account for interactions with solid and liquid phases.
MODEIN	Y	Y	??	MODEIN computes total sediment discharge at a cross section of an alluvial stream having primarily a sand bed from measured hydraulic variables, the concentration and particle-size distribution of the measured suspended sediment, and the particle-size distribution of the bed material.	N	MODEIN only models total solids and does not allow for the water quality parameter inputs.
OTEQ	Y	Y	Y	OTEQ is a a solute transport model that couples One-dimensional Transport with EQUilibrium chemistry. OTEQ is used to characterize the fate and transport of waterborne solutes in streams and rivers. The model is formed by coupling a solute transport model with a chemical equilibrium submodel. The solute transport model is based on OTIS (One-dimensional Transport with Inflow and Storage), a model that considers the physical processes of advection, dispersion, lateral inflow, and transient storage. The equilibrium submodel is based on MINTEQ, a model that considers the speciation and complexation of aqueous species, acid-base reactions, precipitation/dissolution, and sorption.	N	OTEQ is focused on stream and river transport and fate. MINTEQ assesses a limited list of inorganics (metals) and does not include PFAS or constituents that would be considered a surrogate for PFAS.
OTIS	Y	Y	Y	OTIS (One-dimensional Transport with Inflow and Storage), a model that considers the physical processes of advection, dispersion, lateral inflow, and transient storage. The equilibrium submodel is based on MINTEQ, a model that considers the speciation and complexation of aqueous species, acid-base reactions, precipitation/dissolution, and sorption.	N	Like OTEQ, OTIS is focused on stream and river transport and fate and unable to model PFAS parameters.
PRMS	Y	Y	Y	The Precipitation-Runoff Modeling System (PRMS) is a deterministic, distributed-parameter, physical process-based modeling system developed to evaluate the responses of various combinations of climate and land use on streamflow and general watershed hydrology. The primary objectives are: 1. Simulate hydrologic processes, including evaporation, transpiration, runoff, infiltration, and interflow, as determined by the energy and water budgets of the plant canopy, snowpack, and soil zone on the basis of distributed climate information (temperature, precipitation, and solar radiation); 2. Simulate hydrologic water budgets at the watershed scale for temporal scales ranging from days to centuries; 3. Integrate PRMS with other models used for natural resource management or with models from other scientific disciplines; 4. Provide a modular design that allows for selection of alternative hydrologic-process algorithms from the standard PRMS module library.	N	PRMS only models water flow.

Table A-2
 Screening of Surface Water Models for PFAS
 Review of Models for Evaluation of PFAS in Residuals and Biosolids

Model	Public Domain (Y/N)	Supported/Maintained (Y/N)	Peer Reviewed (Y/N)	Summary	Retained (Y/N)	Basis for Rejecting
RRAWFLOW	Y	Y	Y	Rainfall-Response Aquifer and Watershed Flow Model (RRAWFLOW) is a lumped-parameter model that simulates streamflow, springflow, groundwater level, solute transport, or cave drip for a measurement point in response to a system input of precipitation, recharge, or solute injection. For many applications, a simple lumped model, such as RRAWFLOW, simulates the system response with equal accuracy to that of a complex distributed model. Provides professional hydrologists and students with an accessible and versatile tool to assess: hydrologic responses, base flow separation, evaluate hydrologic systems.	N	RRAWFLOW is focused on water flow It does simulate solute transport from point sources but does not account for sediment loading Not intended for runoff loading
seawaveQ	Y	Y	?*	The seawaveQ R package fits a parametric regression model (seawaveQ) to pesticide concentration data from streamwater samples to assess variability and trends. The model incorporates the strong seasonality and high degree of censoring common in pesticide data, and users can incorporate numerous ancillary variables, such as streamflow anomalies. The model is fitted to pesticide data using maximum likelihood methods for censored data and is robust in terms of pesticide, stream location, and degree of censoring of the concentration data. This R package standardizes this methodology for trend analysis, documents the code, and provides help and tutorial information, as well as providing additional utility functions for plotting pesticide and other chemical concentration data.	N	seawaveQ R only models liquid phase and does not account for interactions with solid and liquid phases.
WEBMOD	Y	Y	Y	The Water, Energy, and Biogeochemical Model (WEBMOD) uses the framework of the U.S. Geological Survey (USGS) Modular Modeling System (MMS) to simulate fluxes of water and solutes through watersheds.	Y	N/A
WSPRO	Y	Y	Y	WSPRO computes water-surface profiles for subcritical, critical, or supercritical flow as long as the flow can be reasonably classified as one-dimensional, gradually varied, steady flow. WSPRO can be used to analyze: (1) open-channel flow; (2) flow through bridges; (3) flow through culverts; (4) embankment overflow; and (5) multiple-opening (two or more separate bridge and (or) culvert structures) stream crossings. WSPRO is designated HY-7 in the Federal Highway Administration (FHWA) hydraulics computer program series. A primary objective in developing WSPRO was to provide bridge designers with a highly flexible tool for analyses of alternative bridge openings and (or) embankment configurations. However, WSPRO is equally flexible and suitable for analyses of existing stream crossings. Much of the model's flexibility can be attributed to the data input scheme which, to a great extent, is designed for unformatted, order-independent data. Additional flexibility is provided by propagation of constant data and limited capabilities for synthesizing cross sections. Also, many desirable features from other models were incorporated into WSPRO. The type and quantity of output is to a large extent user-specifiable. Thus WSPRO is a very easy-to-use model, which is generally applicable to water-surface profile analyses for highway design as well as for problems related to flood plain mapping, flood insurance studies, and estimating stage-discharge relationships.	N	WSPRO only analyzes physical water flow characteristics without inputs for water quality parameters.

Notes:

- All models were free and public domain
- GIS = Graphical information system
- HWIR = Hazardous Waste Identification Rules
- N/A = not applicable
- NPS = Non-point source
- PFAS = Per- and polyfluoroalkyl substances
- USEPA = United States Environmental Protection Agency
- USGS = U.S. Geological Survey
- WMU = Waste management unit

Table A-3
Screening of Plant Uptake Models for PFAS
Review of Models for Evaluation of PFAS in Residuals and Biosolids

Model	Model/ Equations in the Public Domain (Y/N)	Peer Reviewed (Y/N)	Summary of Main Model Features & Assumptions	Retained (Y/N)	Basis for Rejecting
Chiou et al. (2001)	Y	Y	<ul style="list-style-type: none"> - Mechanistic model assumes root uptake only - Key input parameters are K_{ow}, weighted average plant fraction lipid, water and carbohydrate content, fraction soil organic carbon - Developed for non-ionic organic compounds 	N	Developed for non-ionized compounds and relies on K_{ow} . Not applicable to PFAS because K_{ow} is not an appropriate sole chemical parameter to model the plant uptake of PFAS
Hung and Mackay (1997)	Y	Y	<ul style="list-style-type: none"> - Dynamic fugacity-based model - Requires several plant- and chemical-specific properties 	N	Intensive data requirements; lack of such data for PFAS
Ryan et al. (1988)	Y	Y	<ul style="list-style-type: none"> - Based on experimental data for non-ionized compounds in barley - Key input parameters are K_{ow}, K_{oc}, and soil parameters including bulk density, water-filled soil porosity, and fraction of organic carbon 	N	Developed for non-ionized compounds and relies on K_{ow} . Not applicable to PFAS because K_{ow} is not an appropriate sole chemical parameter to model the plant uptake of PFAS
Topp et al. (1986)	Y	Y	<ul style="list-style-type: none"> - Regression model based on experimental data on uptake of neutral and ionic organic chemicals by barley and cress seedlings - Only the radioactively labelled carbon concentration was measured 	N	No clear correlation established between concentration of parent chemicals in soil and plants
Trapp and Matthies (1995)	Y	Y	<ul style="list-style-type: none"> - Mechanistic one-compartment mass balance model for leafy vegetables - Key input parameters are plant-specific, chemical-specific, and soil parameters including bulk density, water-filled soil porosity, fraction of organic carbon - Applicable to non-ionized compounds 	N	Only applicable to non-ionized compounds
Trapp 2007	Y	Y	<ul style="list-style-type: none"> - An eight-compartment fruit tree model to predict the concentration of neutral organic chemicals from soil and air into fruits 	N	Only applicable to non-ionized compounds
Trapp 2015	Y	Y	<ul style="list-style-type: none"> - Calibrated for radish with plant- and site-specific data for the uptake of chlorinated organic compounds from soil to radish 	N	Only calibrated for radish and chlorinated organic compounds.
Trapp 2017	Y	Y	<ul style="list-style-type: none"> - Dynamic and steady-state soil-plant uptake models for monovalent organic chemicals such as pesticides and pharmaceuticals - Data intensive. Examples of key input parameters for the steady-state model are K_{ow} for both neutral and ionic species, K_{aw}, partitioning coefficient for adsorption to protein, pKa, ion strength of soil, data on plant morphology 	N	Intensive data requirements; lack of such data for PFAS
Gredelj et al. (2020)	Y	Y	<ul style="list-style-type: none"> - Semi-empirical calibrated for PFAA using empirical data from a previous study (Gredelj et al. 2019) - Examined its applicability to model PFAA concentration in crops from other studies using default inputs for plant parameters such as flow rate of transpiration stream, the mass of plant compartment, and growth rate 	N	Modeled PFAA concentrations for most PFAAs within one order of magnitude of measured; however, intensive data requirements preclude use of this model for screening purposes at this time
Travis and Arms (1988)	Y	Y	<ul style="list-style-type: none"> - Regression model based on K_{ow} and experimental data from various studies 	N	Not applicable to PFAS because K_{ow} is not an appropriate sole chemical parameter to model the plant uptake of PFAS
MMSOILS Model	Y	Y	<ul style="list-style-type: none"> - A multimedia chemical fate, transport, and exposure model that estimates potential human exposure and health risks - Uses transfer factors to model concentration of chemicals in plants 	Y*	-
CSA Plant Uptake Model for Irrigation	Y	Y	<ul style="list-style-type: none"> - Mechanistic model for inorganics - Requires limited number of plant parameters - Uses soil-to-plant transfer factors 	Y*	-

Table A-3
Screening of Plant Uptake Models for PFAS
Review of Models for Evaluation of PFAS in Residuals and Biosolids

Model	Model/ Equations in the Public Domain (Y/N)	Peer Reviewed (Y/N)	Summary of Main Model Features & Assumptions	Retained (Y/N)	Basis for Rejecting
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Notes:
N = No
Y = Yes
Y* = Yes, if PFAS specific transfer factors are available
 K_{aw} = Air/water coefficient
 K_{ow} = n-octanol/water partition coefficient
PFAA = Perfluoroalkyl acid
PFAS = Per- and polyfluoroalkyl substances

APPENDIX B

Summary of Literature-Based Soil to Plants Transfer Factors for Selected PFAS



Table B-1
 Summary of Literature-Based Soil or Solution to Plants Transfer Factors for Selected PFAS
 Review of Models for Evaluation of PFAS in Residuals and Biosolids

Plant	Plant Compartment Analyzed	Plant Species	Plant Category	Type of Study Design	Soil Concentration (ng/g)	Solution Concentration (ng/L)	Equation	Unit	% OC	Transfer Factors														Reference						
										PFBA	PFPeA	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFUnA	PFDaA	PFTTrDA	PFTeDA	PFBS	PFHxS	PFHpS		PFOS	PFOSA	PFDS	PFOS from degradation of PFOSA		
Carrot	total	Chantenay, Daucus carota ssp sativus	Root vegetable	Greenhouse study	PFOA = 495-524; PFOS=432-480; PFOSA=41-562; PFOS (degraded) = 144	-	Cp/Cs	g dw/ g dw	2.30%	-	-	-	-	0.805	-	-	-	-	-	-	-	-	-	-	0.863	0.130	-	0.780	Bizkarguenaga et al. (2016)	
Carrot	total	Chantenay, Daucus carota ssp sativus	Root vegetable	Greenhouse study	PFOA = 553-560; PFOS=402-410; PFOSA=33-530; PFOS (degraded) = 132	-	Cp/Cs	g dw/ g dw	2.30%	-	-	-	-	0.941	-	-	-	-	-	-	-	-	-	-	-	1.071	0.180	-	0.600	Bizkarguenaga et al. (2016)
Carrot Total	total	Nantesa, Daucus carota ssp sativus	Root vegetable	Greenhouse study	PFOA = 439-500; PFOS=324-350; PFOSA=ND-555; PFOS(degraded) =155	-	Cp/Cs	g dw/ g dw	2.30%	-	-	-	-	0.692	-	-	-	-	-	-	-	-	-	-	-	0.829	-	-	0.410	Bizkarguenaga et al. (2016)
Carrot Total	total	Nantesa, Daucus carota ssp sativus	Root vegetable	Greenhouse study	PFOA = 427-470; PFOS=298-320; PFOSA=ND-565; PFOS(degraded) =184	-	Cp/Cs	g dw/ g dw	2.30%	-	-	-	-	1.349	-	-	-	-	-	-	-	-	-	-	-	1.017	-	-	0.430	Bizkarguenaga et al. (2016)
Carrot Total	total	Chantenay, Daucus carota ssp sativus	Root vegetable	Greenhouse study	PFOA =414-425; PFOS=348-480; PFOSA=30-550; PFOS(degraded) = 344	-	Cp/Cs	g dw/ g dw	53.00%	-	-	-	-	0.933	-	-	-	-	-	-	-	-	-	-	-	0.387	-	-	0.250	Bizkarguenaga et al. (2016)
Carrot Total	total	Chantenay, Daucus carota ssp sativus	Root vegetable	Greenhouse study	PFOA =327-390; PFOS=371-380; PFOSA=26-544; PFOS(degraded) =322	-	Cp/Cs	g dw/ g dw	53.00%	-	-	-	-	1.026	-	-	-	-	-	-	-	-	-	-	-	0.463	-	-	0.170	Bizkarguenaga et al. (2016)
Carrot Total	total	Nantesa, Daucus carota ssp sativus	Root vegetable	Greenhouse study	PFOA =470-599; PFOS=401-415; PFOSA=ND-547; PFOS(degraded) = 609	-	Cp/Cs	g dw/ g dw	53.00%	-	-	-	-	0.276	-	-	-	-	-	-	-	-	-	-	-	0.321	-	-	0.280	Bizkarguenaga et al. (2016)
Carrot Total	total	Nantesa, Daucus carota ssp sativus	Root vegetable	Greenhouse study	PFOA = 518-530; PFOS=505-625; PFOSA=ND-551; PFOS(degraded) = 512	-	Cp/Cs	g dw/ g dw	53.00%	-	-	-	-	0.329	-	-	-	-	-	-	-	-	-	-	-	0.181	-	-	0.240	Bizkarguenaga et al. (2016)
Lettuce	total	Golden spring, Lactuca sativa	Leafy green	Greenhouse study	PFOA =540-557; PFOS=481-505; PFOSA=520-530; PFOS (degraded) = 113	-	Cp/Cs	g dw/ g dw	2.30%	-	-	-	-	3.190	-	-	-	-	-	-	-	-	-	-	0.600	0.083	-	0.047	Bizkarguenaga et al. (2016)	
Lettuce	total	Golden spring, Lactuca sativa	Leafy green	Greenhouse study	PFOA =580-633; PFOS=510-555; PFOSA=354-496; PFOS (degraded) = 79	-	Cp/Cs	g dw/ g dw	2.30%	-	-	-	-	2.450	-	-	-	-	-	-	-	-	-	-	-	0.650	0.108	-	0.060	Bizkarguenaga et al. (2016)
Lettuce	total	Golden spring, Lactuca sativa	Leafy green	Greenhouse study	PFOSA=89-500; PFOS (degraded) = 480	-	Cp/Cs	g dw/ g dw	53.00%	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.172	-	0.034	Bizkarguenaga et al. (2016)	
Lettuce	total	Golden spring, Lactuca sativa	Leafy green	Greenhouse study	PFOSA=134-510; PFOS (degraded) = 477	-	Cp/Cs	g dw/ g dw	53.00%	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.109	-	0.023	Bizkarguenaga et al. (2016)	
Corn	stover	Zea mays	Animal feed	Field study	Chemical specific, 2 x soil, <0.1-6.12	-	Cp/Cs	g dw/ g dw	2.34%	64.800	41.100	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Blaine et al. (2013)	
Lettuce	Leaves	Lactuca sativa	Leafy green	Greenhouse study	Chemical specific, 0.54-93.45	-	Cp/Cs	g dw/ g dw	2.24%	56.800	20.400	9.900	2.660	2.520	2.850	0.520	-	-	-	-	4.220	7.560	6.570	1.670	-	-	-	-	Blaine et al. (2013)	
Lettuce	leaves	Lactuca sativa	Leafy green	Field study	Chemical specific, 4 x soil, 0.16-13.91	-	Cp/Cs	g dw/ g dw	3.51%	40.000	16.300	-	-	-	-	-	-	-	-	2.020	1.510	-	0.100	-	-	-	-	-	Blaine et al. (2013)	
Lettuce	leaves	Lactuca sativa	Leafy green	Greenhouse study	Chemical specific, 0.21-319.49	-	Cp/Cs	g dw/ g dw	6.34%	28.400	10.200	11.700	3.330	1.340	0.770	0.340	-	-	-	-	14.500	1.080	1.030	0.320	-	0.190	-	-	Blaine et al. (2013)	

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Plant	Plant Compartment Analyzed	Plant Species	Plant Category	Type of Study Design	Soil Concentration (ng/g)	Solution Concentration (ng/L)	Equation	Unit	% OC	Transfer Factors														Reference				
										PFBA	PFPeA	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFUnA	PFDaA	PFTTrDA	PFTeDA	PFBS	PFHxS	PFHpS		PFOS	PFOSA	PFDS	PFOS from degradation of PFOSA
Tomato	fruit	Lycopersicon lycopersicum	Fruit	Greenhouse study	Chemical specific, 0.54-93.45	-	Cp/Cs	g dw/ g dw	2.24%	12.200	17.100	2.900	0.860	0.110	-	-	-	-	-	-	0.420	0.500	-	-	-	-	Blaine et al. (2013)	
Tomato	fruit	Lycopersicon lycopersicum	Fruit	Field study	Chemical specific, 4 x soil, 0.16-13.91	-	Cp/Cs	g dw/ g dw	3.51%	18.200	14.900	6.840	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Blaine et al. (2013)	
Celery	root	Apium graveolens var. dulce	Other - vegetative compartment	Greenhouse study	Chemical specific, <0.5 -93.45	-	Croot/Cpw	ml/ g dw	-	29.320	2.020	2.180	2.820	2.460	9.720	21.720	-	-	-	-	3.480	12.500	-	59.650	-	-	-	Blaine et al. (2014a)
Celery	root	Apium graveolens var. dulce	Other - vegetative compartment	Greenhouse study	Chemical specific, <0.5 -93.45	-	Croot/Cs	g dw/ g dw	2.24%	17.270	3.840	4.770	2.960	1.420	1.900	1.060	-	-	-	-	2.520	4.980	-	4.220	-	-	-	Blaine et al. (2014a)
Celery	shoot	Apium graveolens var. dulce	Other vegetables	Greenhouse study	Chemical specific, <0.5 -93.45	-	Cshoot/Cs	g dw/ g dw	2.24%	49.490	12.810	11.910	2.510	0.710	0.690	0.320	-	-	-	-	2.210	2.310	-	1.390	-	-	-	Blaine et al. (2014a)
Pea	root	Pisum sativum var. macrocarpon	Other - vegetative compartment	Greenhouse study	Chemical specific, <0.5 -93.45	-	Croot/Cpw	ml/ g dw	-	3.280	0.270	0.470	1.480	1.380	8.750	29.170	-	-	-	-	1.220	-	-	33.740	-	-	-	Blaine et al. (2014a)
Pea	fruit	Pisum sativum var. macrocarpon	Legume	Greenhouse study	Chemical specific, <0.5 -93.45	-	Cfruit/Cs	g dw/ g dw	2.24%	32.070	3.970	1.470	0.180	0.030	0.070	-	-	-	-	-	0.330	0.170	-	0.030	-	-	-	Blaine et al. (2014a)
Pea	root	Pisum sativum var. macrocarpon	Other - vegetative compartment	Greenhouse study	Chemical specific, <0.5 -93.45	-	Croot/Cs	g dw/ g dw	2.24%	1.930	0.510	1.040	1.550	0.790	1.710	1.430	-	-	-	-	0.890	-	-	2.390	-	-	-	Blaine et al. (2014a)
Pea	shoot	Pisum sativum var. macrocarpon	Other - vegetative compartment	Greenhouse study	Chemical specific, <0.5 -93.45	-	Cshoot/Cs	g dw/ g dw	2.24%	10.890	4.520	3.460	1.250	0.520	0.440	0.150	-	-	-	-	4.120	4.330	-	1.240	-	-	-	Blaine et al. (2014a)
Radish	root	Raphanus sativus	Root vegetable	Greenhouse study	Chemical specific, <0.5 -93.45	-	Croot/Cpw	ml/ g dw	-	4.960	0.500	0.520	0.760	1.480	6.790	8.940	-	-	-	-	1.760	5.160	-	9.910	-	-	-	Blaine et al. (2014a)
Radish	root	Raphanus sativus	Root vegetable	Greenhouse study	Chemical specific, <0.5 -93.45	-	Croot/Cs	g dw/ g dw	2.24%	2.920	0.950	1.150	0.800	0.850	1.320	0.440	-	-	-	-	1.270	2.050	-	0.700	-	-	-	Blaine et al. (2014a)
Radish	shoot	Raphanus sativus	Other - vegetative compartment	Greenhouse study	Chemical specific, <0.5 -93.45	-	Cshoot/Cs	g dw/ g dw	2.24%	13.820	4.160	3.860	5.500	7.600	5.310	1.100	-	-	-	-	3.380	7.460	-	3.740	-	-	-	Blaine et al. (2014a)
Tomato	root	Lycopersicon lycopersicum	Other - vegetative compartment	Greenhouse study	Chemical specific, <0.5 -93.45	-	Croot/Cpw	ml/ g dw	-	8.560	0.400	0.660	1.800	1.660	9.870	37.860	-	-	-	-	0.980	4.400	-	64.020	-	-	-	Blaine et al. (2014a)
Tomato	fruit	Lycopersicon lycopersicum	Fruit	Greenhouse study	Chemical specific, <0.5 -93.45	-	Cfruit/Cs	g dw/ g dw	2.24%	12.160	17.060	2.900	0.860	0.110	-	-	-	-	-	-	0.420	0.500	-	-	-	-	Blaine et al. (2014a)	
Tomato	root	Lycopersicon lycopersicum	Other - vegetative compartment	Greenhouse study	Chemical specific, <0.5 -93.45	-	Croot/Cs	g dw/ g dw	2.24%	5.040	0.760	1.450	1.880	0.960	1.920	1.850	-	-	-	-	0.710	1.750	-	4.530	-	-	-	Blaine et al. (2014a)
Tomato	shoot	Lycopersicon lycopersicum	Other - vegetative compartment	Greenhouse study	Chemical specific, <0.5 -93.45	-	Cshoot/Cs	g dw/ g dw	2.24%	26.030	8.570	8.930	3.790	2.420	2.350	1.430	-	-	-	-	3.650	5.600	-	4.240	-	-	-	Blaine et al. (2014a)
Lettuce	leaves	Lactuca sativa	Leafy green	Greenhouse study	Estimated based on measured Kd values	10 ug/L	Cf/Cw x Kd	g dw/ g dw	0.40%	1560.000	819.000	415.000	122.000	34.900	11.500	-	-	-	-	-	102.000	46.200	-	6.490	-	-	-	Blaine et al. (2014b)
Lettuce	leaves	Lactuca sativa	Leafy green	Greenhouse study	Estimated based on measured Kd values	10 ug/L	Cf/Cw x Kd	g dw/ g dw	2.00%	3390.000	1300.000	321.000	34.700	4.300	1.650	-	-	-	-	-	316.000	17.700	-	4.810	-	-	-	Blaine et al. (2014b)
Lettuce	leaves	Lactuca sativa	Leafy green	Greenhouse study	Estimated based on measured Kd values	10 ug/L	Cf/Cw x Kd	g dw/ g dw	6.00%	767.000	314.000	71.800	7.260	1.180	0.938	-	-	-	-	-	58.300	3.520	-	0.759	-	-	-	Blaine et al. (2014b)
Strawberry	fruit	Fragaria ananassa	Fruit	Greenhouse study	Estimated based on measured Kd values	10 ug/L	Cf/Cw x Kd	g dw/ g dw	0.40%	203.000	243.000	34.500	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Blaine et al. (2014b)	
Perennial Ryegrass (4th cutting)	grass	Not available	Animal feed	Laboratory study, experimental pot	1000	-	Cgrass/Cs	g dw/ g dw	NA	-	-	-	-	7.520	-	-	-	-	-	-	-	-	-	0.470	-	-	-	calculated based on data from Stahl et al. (2009)
Perennial Ryegrass (4th cutting)	grass	Not available	Animal feed	Laboratory study, experimental pot	250	-	Cgrass/Cs	g dw/ g dw	NA	-	-	-	-	6.200	-	-	-	-	-	-	-	-	-	0.352	-	-	-	calculated based on data from Stahl et al. (2009)
Potato	peels	Not available	Other - vegetative compartment	Laboratory study, experimental pot	10000	-	Cpeels/Cs	g dw/ gww	NA	-	-	-	-	0.002	-	-	-	-	-	-	-	-	0.009	-	-	-	calculated based on data from Stahl et al. (2009)	
Potato	tuber	Not available	Root vegetable	Laboratory study, experimental pot	10000	-	Ctuber/Cs	g dw/ gww	NA	-	-	-	-	0.001	-	-	-	-	-	-	-	-	0.001	-	-	-	calculated based on data from Stahl et al. (2009)	
Cabbage	head	Brassica oleracea convar. capitata var. alba	Leafy green	Greenhouse study	-	10	Chead/Cw	ml/ g ww	-	8.365	9.302	3.563	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Felizeter et al. (2014), Calculated by Arcadis	
Cabbage	head	Brassica oleracea convar. capitata var. alba	Leafy green	Greenhouse study	-	100	Chead/Cw	ml/ g ww	-	4.406	4.966	1.778	0.351	0.382	-	-	-	-	-	-	0.404	0.274	-	-	-	-	Felizeter et al. (2014), Calculated by Arcadis	
Cabbage	head	Brassica oleracea convar. capitata var. alba	Leafy green	Greenhouse study	-	500	Chead/Cw	ml/ g ww	-	3.209	3.152	1.043	0.206	0.381	0.144	0.125	0.064	-	-	-	0.310	0.226	-	0.142	-	-	-	Felizeter et al. (2014), Calculated by Arcadis

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Plant	Plant Compartment Analyzed	Plant Species	Plant Category	Type of Study Design	Soil Concentration (ng/g)	Solution Concentration (ng/L)	Equation	Unit	% OC	Transfer Factors															Reference			
										PFBA	PFPeA	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFUnA	PFDoA	PFTTrDA	PFTeDA	PFBS	PFHxS	PFHpS	PFOS		PFOSA	PFDS	PFOS from degradation of PFOSA
Cabbage	head	Brassica oleracea convar. capitata var. alba	Leafy green	Greenhouse study	-	1000	Chead/Cw	ml/ g ww	-	5.491	5.564	1.819	0.263	0.328	0.187	0.179	0.094	-	-	-	0.491	0.231	-	0.199	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Cabbage	leaf	Brassica oleracea convar. capitata var. alba	Other - vegetative compartment	Greenhouse study	-	10	Cleaf/Cw	ml/ g ww	-	30.769	13.953	8.750	8.594	9.608	8.075	7.413	-	-	-	-	10.553	7.559	-	5.789	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Cabbage	leaf	Brassica oleracea convar. capitata var. alba	Other - vegetative compartment	Greenhouse study	-	100	Cleaf/Cw	ml/ g ww	-	6.993	5.374	4.944	6.791	8.727	6.000	5.131	2.403	-	-	-	10.155	8.306	-	6.863	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Cabbage	leaf	Brassica oleracea convar. capitata var. alba	Other - vegetative compartment	Greenhouse study	-	500	Cleaf/Cw	ml/ g ww	-	6.047	4.348	4.065	6.106	8.802	8.675	7.864	2.433	0.590	-	-	10.445	9.419	-	9.340	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Cabbage	leaf	Brassica oleracea convar. capitata var. alba	Other - vegetative compartment	Greenhouse study	-	1000	Cleaf/Cw	ml/ g ww	-	8.225	5.985	5.613	7.829	10.520	9.507	9.450	3.483	0.599	-	-	11.935	10.162	-	8.350	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Cabbage	root	Brassica oleracea convar. capitata var. alba	Other - vegetative compartment	Greenhouse study	-	10	Cr/Cw	ml/ g ww	-	-	10.078	17.500	22.656	80.392	185.841	335.664	307.806	201.278	240.700	226.044	15.075	46.457	-	233.533	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Cabbage	root	Brassica oleracea convar. capitata var. alba	Other - vegetative compartment	Greenhouse study	-	100	Cr/Cw	ml/ g ww	-	4.755	6.327	10.611	14.701	36.636	94.095	204.057	221.629	170.213	184.362	263.415	19.896	37.984	-	173.077	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Cabbage	root	Brassica oleracea convar. capitata var. alba	Other - vegetative compartment	Greenhouse study	-	500	Cr/Cw	ml/ g ww	-	5.496	4.189	5.624	8.746	19.782	47.201	118.182	164.973	102.655	167.769	168.571	11.996	21.129	-	101.587	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Cabbage	root	Brassica oleracea convar. capitata var. alba	Other - vegetative compartment	Greenhouse study	-	1000	Cr/Cw	ml/ g ww	-	5.621	5.505	8.618	11.971	24.470	48.867	108.005	173.427	78.144	115.385	119.139	17.568	26.644	-	109.379	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Cabbage	stem	Brassica oleracea convar. capitata var. alba	Other - vegetative compartment	Greenhouse study	-	10	Cshoot/Cw	ml/ g ww	-	-	2.868	-	-	2.647	-	-	-	-	-	-	-	-	-	-	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Cabbage	stem	Brassica oleracea convar. capitata var. alba	Other - vegetative compartment	Greenhouse study	-	100	Cshoot/Cw	ml/ g ww	-	2.587	1.769	1.778	0.896	1.909	2.286	4.296	5.073	3.191	-	-	0.451	1.210	-	2.990	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Cabbage	stem	Brassica oleracea convar. capitata var. alba	Other - vegetative compartment	Greenhouse study	-	500	Cshoot/Cw	ml/ g ww	-	1.928	0.957	0.591	0.383	1.615	2.649	6.409	7.727	2.891	0.579	-	0.321	0.935	-	3.962	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Cabbage	stem	Brassica oleracea convar. capitata var. alba	Other - vegetative compartment	Greenhouse study	-	1000	Cshoot/Cw	ml/ g ww	-	3.153	1.876	1.311	0.607	1.734	2.916	6.368	11.343	3.383	0.582	-	0.502	1.221	-	3.641	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	fruit	Solanum lycopersicum var. MoneyMaker	Fruit	Greenhouse study	-	10	Cfruit/Cw	ml/ g ww	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	fruit	Solanum lycopersicum var. MoneyMaker	Fruit	Greenhouse study	-	100	Cfruit/Cw	ml/ g ww	-	4.234	4.755	2.606	0.395	0.274	-	-	-	-	-	-	0.222	-	-	-	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	fruit	Solanum lycopersicum var. MoneyMaker	Fruit	Greenhouse study	-	1000	Cfruit/Cw	ml/ g ww	-	4.174	4.656	2.134	0.443	0.273	0.072	0.030	-	-	-	-	0.150	0.046	-	-	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	fruit	Solanum lycopersicum var. MoneyMaker	Fruit	Greenhouse study	-	10000	Cfruit/Cw	ml/ g ww	-	3.551	4.645	2.390	0.863	0.330	0.100	0.048	0.006	-	-	-	0.145	0.065	-	0.031	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	leaf	Solanum lycopersicum var. MoneyMaker	Other - vegetative compartment	Greenhouse study	-	10	Cleaf/Cw	ml/ g ww	-	35.246	7.463	17.763	44.167	47.571	24.731	21.021	-	-	-	-	35.326	23.077	-	24.457	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	leaf	Solanum lycopersicum var. MoneyMaker	Other - vegetative compartment	Greenhouse study	-	100	Cleaf/Cw	ml/ g ww	-	15.912	6.154	15.152	28.760	33.491	29.330	20.175	6.410	2.521	-	-	38.667	29.823	-	28.125	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	leaf	Solanum lycopersicum var. MoneyMaker	Other - vegetative compartment	Greenhouse study	-	1000	Cleaf/Cw	ml/ g ww	-	31.982	8.465	30.885	61.885	83.789	66.734	47.292	16.766	2.340	0.505	0.324	69.961	45.530	-	40.247	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	leaf	Solanum lycopersicum var. MoneyMaker	Other - vegetative compartment	Greenhouse study	-	10000	Cleaf/Cw	ml/ g ww	-	24.560	9.686	14.168	53.721	55.642	57.814	45.616	12.605	1.408	0.280	0.132	27.767	26.128	-	40.979	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	root	Solanum lycopersicum var. MoneyMaker	Other - vegetative compartment	Greenhouse study	-	10	Cr/Cw	ml/ g ww	-	-	-	4.013	4.000	6.680	45.161	147.147	176.718	224.080	149.028	206.468	-	12.821	-	98.746	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	root	Solanum lycopersicum var. MoneyMaker	Other - vegetative compartment	Greenhouse study	-	100	Cr/Cw	ml/ g ww	-	1.022	1.259	3.879	3.876	16.321	60.468	122.932	296.474	218.487	191.091	221.990	7.444	23.540	-	103.097	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	root	Solanum lycopersicum var. MoneyMaker	Other - vegetative compartment	Greenhouse study	-	1000	Cr/Cw	ml/ g ww	-	1.074	1.385	2.398	3.008	10.547	49.696	105.174	222.552	112.462	121.212	126.389	5.114	11.258	-	74.313	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	root	Solanum lycopersicum var. MoneyMaker	Other - vegetative compartment	Greenhouse study	-	10000	Cr/Cw	ml/ g ww	-	0.542	1.004	1.149	2.246	6.174	31.958	82.771	266.707	13.909	19.307	24.583	4.186	6.848	-	54.441	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	stem	Solanum lycopersicum var. MoneyMaker	Other - vegetative compartment	Greenhouse study	-	10	Cshoot/Cw	ml/ g ww	-	2.869	-	2.763	4.500	9.312	9.032	16.517	14.025	7.692	-	-	3.098	3.932	-	10.658	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	stem	Solanum lycopersicum var. MoneyMaker	Other - vegetative compartment	Greenhouse study	-	100	Cshoot/Cw	ml/ g ww	-	1.533	2.168	2.848	5.814	8.491	8.395	10.902	7.853	3.866	1.826	-	3.111	4.867	-	13.542	-	-	-	Felizeter et al. (2014), Calculated by Arcadis

Table B-1
Summary of Literature-Based Soil or Solution to Plants Transfer Factors for Selected PFAS
Review of Models for Evaluation of PFAS in Residuals and Biosolids

Plant	Plant Compartment Analyzed	Plant Species	Plant Category	Type of Study Design	Soil Concentration (ng/g)	Solution Concentration (ng/L)	Equation	Unit	% OC	Transfer Factors															Reference			
										PFBA	PFPeA	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFUnA	PFDoA	PFTTrDA	PFTeDA	PFBS	PFHxS	PFHpS	PFOS		PFOSA	PFDS	PFOS from degradation of PFOSA
Tomato	stem	Solanum lycopersicum var. MoneyMaker	Other - vegetative compartment	Greenhouse study	-	1000	Cshoot/Cw	ml/ g ww	-	1.794	1.363	1.620	3.910	6.807	9.381	12.515	13.412	6.079	1.859	0.417	1.138	4.553	-	7.559	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	stem	Solanum lycopersicum var. MoneyMaker	Other - vegetative compartment	Greenhouse study	-	10000	Cshoot/Cw	ml/ g ww	-	1.124	1.428	2.013	4.274	7.945	11.480	15.328	15.832	3.206	1.020	0.292	1.952	3.213	-	8.291	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	twig	Solanum lycopersicum var. MoneyMaker	Other - vegetative compartment	Greenhouse study	-	10	Ctwig/Cw	ml/ g ww	-	-	-	5.461	4.833	8.502	11.828	8.709	16.830	-	-	-	9.239	3.590	-	7.065	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	twig	Solanum lycopersicum var. MoneyMaker	Other - vegetative compartment	Greenhouse study	-	100	Ctwig/Cw	ml/ g ww	-	6.788	3.007	4.364	5.736	8.774	8.714	9.649	6.090	1.849	1.826	-	9.333	6.195	-	6.771	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	twig	Solanum lycopersicum var. MoneyMaker	Other - vegetative compartment	Greenhouse study	-	1000	Ctwig/Cw	ml/ g ww	-	10.060	5.050	6.842	9.672	11.230	12.069	14.079	11.617	3.131	0.687	0.231	10.161	5.381	-	7.541	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Tomato	twig	Solanum lycopersicum var. MoneyMaker	Other - vegetative compartment	Greenhouse study	-	10000	Ctwig/Cw	ml/ g ww	-	7.331	3.740	4.378	6.822	9.774	11.997	17.658	10.519	2.815	0.742	0.195	5.426	3.651	-	9.413	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	leaf	Cucurbita pepo var. Black Beauty	Other - vegetative compartment	Greenhouse study	-	10	Cleaf/Cw	ml/ g ww	-	33.540	19.643	9.184	7.947	15.574	18.349	22.528	7.576	-	-	-	21.267	16.438	-	18.605	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	leaf	Cucurbita pepo var. Black Beauty	Other - vegetative compartment	Greenhouse study	-	100	Cleaf/Cw	ml/ g ww	-	15.057	12.486	8.900	10.855	16.613	16.303	15.484	6.502	0.896	-	-	21.096	17.902	-	20.909	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	leaf	Cucurbita pepo var. Black Beauty	Other - vegetative compartment	Greenhouse study	-	500	Cleaf/Cw	ml/ g ww	-	16.219	11.924	10.959	11.036	17.667	17.247	13.671	5.957	0.565	0.119	-	20.541	17.867	-	18.017	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	leaf	Cucurbita pepo var. Black Beauty	Other - vegetative compartment	Greenhouse study	-	1000	Cleaf/Cw	ml/ g ww	-	20.541	13.862	10.418	11.291	21.829	19.874	17.433	5.854	0.559	0.158	-	19.215	19.129	-	14.744	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	twig	Cucurbita pepo var. Black Beauty	Other - vegetative compartment	Greenhouse study	-	10	Ctwig/Cw	ml/ g ww	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	twig	Cucurbita pepo var. Black Beauty	Other - vegetative compartment	Greenhouse study	-	100	Ctwig/Cw	ml/ g ww	-	1.552	1.098	1.244	1.250	2.581	3.193	4.624	3.641	1.258	-	-	0.658	1.189	-	1.816	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	twig	Cucurbita pepo var. Black Beauty	Other - vegetative compartment	Greenhouse study	-	500	Ctwig/Cw	ml/ g ww	-	1.400	1.381	1.693	2.046	3.283	3.997	5.680	5.499	1.215	0.172	-	0.838	1.427	-	2.217	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	twig	Cucurbita pepo var. Black Beauty	Other - vegetative compartment	Greenhouse study	-	1000	Ctwig/Cw	ml/ g ww	-	2.086	2.176	2.089	2.272	3.184	4.417	5.733	5.000	1.060	0.109	-	0.692	1.352	-	1.652	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	fruit	Cucurbita pepo var. Black Beauty	Other vegetables	Greenhouse study	-	10	Cfruit/Cw	ml/ g ww	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	fruit	Cucurbita pepo var. Black Beauty	Other vegetables	Greenhouse study	-	100	Cfruit/Cw	ml/ g ww	-	0.690	0.925	0.718	0.461	0.242	0.420	-	-	-	-	-	0.307	-	-	0.318	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	fruit	Cucurbita pepo var. Black Beauty	Other vegetables	Greenhouse study	-	500	Cfruit/Cw	ml/ g ww	-	0.712	0.897	0.802	0.511	0.283	0.348	0.345	0.178	-	-	-	0.324	0.274	-	0.267	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	fruit	Cucurbita pepo var. Black Beauty	Other vegetables	Greenhouse study	-	1000	Cfruit/Cw	ml/ g ww	-	0.798	0.859	0.851	0.508	0.250	0.397	0.289	0.112	-	-	-	0.346	0.229	-	0.209	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	root	Cucurbita pepo var. Black Beauty	Other - vegetative compartment	Greenhouse study	-	10	Cr/Cw	ml/ g ww	-	-	5.952	7.143	10.596	30.328	81.651	236.546	345.455	319.224	174.853	614.706	9.502	21.918	-	130.233	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	root	Cucurbita pepo var. Black Beauty	Other - vegetative compartment	Greenhouse study	-	100	Cr/Cw	ml/ g ww	-	2.184	3.699	6.268	11.118	29.516	56.639	125.806	236.671	257.862	155.131	746.914	11.360	27.972	-	101.364	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	root	Cucurbita pepo var. Black Beauty	Other - vegetative compartment	Greenhouse study	-	500	Cr/Cw	ml/ g ww	-	1.995	5.407	7.828	10.888	27.667	61.194	110.751	301.887	145.198	141.379	430.688	12.532	28.963	-	115.422	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	root	Cucurbita pepo var. Black Beauty	Other - vegetative compartment	Greenhouse study	-	1000	Cr/Cw	ml/ g ww	-	1.661	2.884	4.447	9.386	24.935	46.251	92.620	232.493	100.000	114.008	196.314	8.901	14.623	-	87.950	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	stem	Cucurbita pepo var. Black Beauty	Other - vegetative compartment	Greenhouse study	-	10	Cshoot/Cw	ml/ g ww	-	-	-	7.143	7.285	10.656	16.514	12.516	7.576	-	-	-	-	5.548	-	6.871	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	stem	Cucurbita pepo var. Black Beauty	Other - vegetative compartment	Greenhouse study	-	100	Cshoot/Cw	ml/ g ww	-	-	-	5.694	7.632	10.000	10.504	8.172	6.372	2.673	-	-	1.491	4.825	-	9.091	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	stem	Cucurbita pepo var. Black Beauty	Other - vegetative compartment	Greenhouse study	-	500	Cshoot/Cw	ml/ g ww	-	0.583	1.570	4.540	8.371	9.917	10.017	8.621	7.089	2.119	0.272	0.164	1.243	3.963	-	6.293	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Zucchini	stem	Cucurbita pepo var. Black Beauty	Other - vegetative compartment	Greenhouse study	-	1000	Cshoot/Cw	ml/ g ww	-	0.934	2.288	5.071	8.059	10.267	10.623	10.107	7.605	2.321	0.409	0.140	1.258	3.412	-	4.915	-	-	-	Felizeter et al. (2014), Calculated by Arcadis
Maize	grain	Zea mays	Grains	Laboratory study, experimental pot	1000	-	Cgrain/Cs	g dw/ g dw	0.27%	0.229	0.380	0.216	0.027	0.002	-	-	-	-	-	-	0.005	-	-	-	-	-	Krippner et al. (2015)	

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Plant	Plant Compartment Analyzed	Plant Species	Plant Category	Type of Study Design	Soil Concentration (ng/g)	Solution Concentration (ng/L)	Equation	Unit	% OC	Transfer Factors														Reference					
										PFBA	PFPeA	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFUnA	PFDaA	PFTTrDA	PFTeDA	PFBS	PFHxS	PFHpS		PFOS	PFOSA	PFDS	PFOS from degradation of PFOSA	
Maize	grain	Zea mays	Grains	Laboratory study, experimental pot	250	-	Cgrain/Cs	g dw/ g dw	0.27%	0.133	0.366	0.123	0.016	-	-	-	-	-	-	-	0.008	-	-	-	-	-	-	Krippner et al. (2015)	
Maize	straw	Zea mays	Animal feed	Laboratory study, experimental pot	1000	-	Cstraw/Cs	g dw/ g dw	0.27%	35.230	8.330	2.820	1.670	0.650	0.160	0.040	-	-	-	-	-	1.840	0.850	-	0.620	-	-	-	Krippner et al. (2015)
Maize	straw	Zea mays	Animal feed	Laboratory study, experimental pot	250	-	Cstraw/Cs	g dw/ g dw	0.27%	63.640	14.680	3.190	1.410	0.560	0.120	0.030	-	-	-	-	-	3.850	0.840	-	0.320	-	-	-	Krippner et al. (2015)
Carrot	edible part	Daucus carota ssp. Sativus	Root vegetable	Greenhouse study	Tub 1, PFOA = 681, PFOS = 10	-	Cp/Cs	g dm soil/ g ww	3% DM	-	-	-	-	0.050	-	-	-	-	-	-	-	-	-	-	0.050	-	-	-	Lechner and Knapp (2011)
Carrot	edible part	Daucus carota ssp. Sativus	Root vegetable	Greenhouse study	Tub 2, PFOA = 676, PFOS = 458	-	Cp/Cs	g dm soil/ g ww	3% DM	-	-	-	-	0.050	-	-	-	-	-	-	-	-	-	-	0.040	-	-	-	Lechner and Knapp (2011)
Carrot	peels	Daucus carota ssp. Sativus	Root vegetable	Greenhouse study	Tub 1, PFOA = 681, PFOS = 10	-	Cp/Cs	g dm soil/ g ww	3% DM	-	-	-	-	0.040	-	-	-	-	-	-	-	-	-	-	0.030	-	-	-	Lechner and Knapp (2011)
Carrot	peels	Daucus carota ssp. Sativus	Root vegetable	Greenhouse study	Tub 2, PFOA = 676, PFOS = 458	-	Cp/Cs	g dm soil/ g ww	3% DM	-	-	-	-	0.040	-	-	-	-	-	-	-	-	-	-	0.040	-	-	-	Lechner and Knapp (2011)
Carrot	vegetative compartment	Daucus carota ssp. Sativus	Other - vegetative compartment	Greenhouse study	Tub 1, PFOA = 681, PFOS = 10	-	Cp/Cs	g dm soil/ g ww	3% DM	-	-	-	-	0.530	-	-	-	-	-	-	-	-	-	-	0.320	-	-	-	Lechner and Knapp (2011)
Carrot	vegetative compartment	Daucus carota ssp. Sativus	Other - vegetative compartment	Greenhouse study	Tub 2, PFOA = 676, PFOS = 458	-	Cp/Cs	g dm soil/ g ww	3% DM	-	-	-	-	0.530	-	-	-	-	-	-	-	-	-	-	0.430	-	-	-	Lechner and Knapp (2011)
Cucumber, unpeeled	edible part	Cucumis Sativus	Other vegetables	Greenhouse study	Tub 1, PFOA = 406, PFOS = 10	-	Cp/Cs	g dm soil/ g ww	3% DM	-	-	-	-	0.030	-	-	-	-	-	-	-	-	-	-	0.000	-	-	-	Lechner and Knapp (2011)
Cucumber, unpeeled	edible part	Cucumis Sativus	Other vegetables	Greenhouse study	Tub 2, PFOA = 805, PFOS = 556	-	Cp/Cs	g dm soil/ g ww	3% DM	-	-	-	-	0.030	-	-	-	-	-	-	-	-	-	-	<0.01	-	-	-	Lechner and Knapp (2011)
Cucumber, unpeeled	vegetative compartment	Cucumis Sativus	Other vegetables	Greenhouse study	Tub 1, PFOA = 406, PFOS = 10	-	Cp/Cs	g dm soil/ g ww	3% DM	-	-	-	-	0.760	-	-	-	-	-	-	-	-	-	-	0.120	-	-	-	Lechner and Knapp (2011)
Cucumber, unpeeled	vegetative compartment	Cucumis Sativus	Other vegetables	Greenhouse study	Tub 2, PFOA = 805, PFOS = 556	-	Cp/Cs	g dm soil/ g ww	3% DM	-	-	-	-	0.990	-	-	-	-	-	-	-	-	-	-	0.210	-	-	-	Lechner and Knapp (2011)
Potato	peels	Solanum tuberosum	Root vegetable	Greenhouse study	Tub 1, PFOA = 276, PFOS = 15	-	Cp/Cs	g dm soil/ g ww	3% DM	-	-	-	-	0.030	-	-	-	-	-	-	-	-	-	-	0.020	-	-	-	Lechner and Knapp (2011)
Potato	peels	Solanum tuberosum	Root vegetable	Greenhouse study	Tub 2, PFOA = 795, PFOS = 317	-	Cp/Cs	g dm soil/ g ww	3% DM	-	-	-	-	0.020	-	-	-	-	-	-	-	-	-	-	0.050	-	-	-	Lechner and Knapp (2011)
Potato	edible part	Solanum tuberosum	Root vegetable	Greenhouse study	Tub 1, PFOA = 276, PFOS = 15	-	Cp/Cs	g dm soil/ g ww	3% DM	-	-	-	-	0.010	-	-	-	-	-	-	-	-	-	-	0.000	-	-	-	Lechner and Knapp (2011)
Potato	edible part	Solanum tuberosum	Root vegetable	Greenhouse study	Tub 2, PFOA = 795, PFOS = 317	-	Cp/Cs	g dm soil/ g ww	3% DM	-	-	-	-	0.010	-	-	-	-	-	-	-	-	-	-	<0.01	-	-	-	Lechner and Knapp (2011)
Potato	vegetative compartment	Solanum tuberosum	Other - vegetative compartment	Greenhouse study	Tub 1, PFOA = 276, PFOS = 15	-	Cp/Cs	g dm soil/ g ww	3% DM	-	-	-	-	0.380	-	-	-	-	-	-	-	-	-	-	0.270	-	-	-	Lechner and Knapp (2011)
Potato	vegetative compartment	Solanum tuberosum	Other - vegetative compartment	Greenhouse study	Tub 2, PFOA = 795, PFOS = 317	-	Cp/Cs	g dm soil/ g ww	3% DM	-	-	-	-	0.420	-	-	-	-	-	-	-	-	-	-	0.450	-	-	-	Lechner and Knapp (2011)
Corn	leaf	Zea mays	Other - vegetative compartment	Laboratory study, experimental pot	chemical specific	-	Cp/Cs	g dw/ g dw	-	-	-	-	-	-	-	-	-	-	-	-	4.000	9.390	-	0.800	-	-	-	Navarro et al. (2017)	
Corn	root	Zea mays	Other - vegetative compartment	Laboratory study, experimental pot	chemical specific	-	Cp/Cs	g dw/ g dw	-	-	-	-	-	-	-	-	-	-	-	-	5.000	2.620	-	8.820	-	-	-	Navarro et al. (2017)	
Spinach	total	Spinacia oleracea	Leafy green	Laboratory study, experimental pot	Chemical specific, Treatment 1, 0.1-2.73	-	Cp/Cs	g dw/ g dw	33.21%	-	1.080	-	-	1.630	-	-	-	-	-	-	-	-	-	-	3.820	-	-	-	Navarro et al. (2017)
Spinach	total	Spinacia oleracea	Leafy green	Laboratory study, experimental pot	Chemical Specific, Treatment 2, ND - 0.23	-	Cp/Cs	g dw/ g dw	11.55%	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	4.470	-	-	-	Navarro et al. (2017)
Tomato	fruit	Solanum lycopersicum L.	Fruit	Laboratory study, experimental pot	Chemical specific, Treatment 1, 0.1-2.73	-	Cp/Cs	g dw/ g dw	33.21%	30.870	31.220	3.640	0.910	0.080	-	0.020	-	-	-	-	-	-	-	-	0.060	-	-	-	Navarro et al. (2017)
Tomato	leaf	Solanum lycopersicum L.	Other - vegetative compartment	Laboratory study, experimental pot	Chemical specific, Treatment 1, 0.1-2.73	-	Cp/Cs	g dw/ g dw	33.21%	94.410	27.840	6.910	-	3.550	0.280	-	-	-	-	-	-	-	-	-	1.240	-	-	-	Navarro et al. (2017)
Tomato	root	Solanum lycopersicum L.	Other - vegetative compartment	Laboratory study, experimental pot	Chemical specific, Treatment 1, 0.1-2.73	-	Cp/Cs	g dw/ g dw	33.21%	-	6.120	1.000	5.330	4.370	4.530	2.700	-	-	-	-	-	-	-	-	2.250	-	-	-	Navarro et al. (2017)

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Tomato	stem	Solanum lycopersicum L.	Other - vegetative compartment	Laboratory study, experimental pot	Chemical specific, Treatment 1, 0.1-2.73	-	Cp/Cs	g dw/ g dw	33.21%	15.350	11.670	1.770	-	0.550	-	0.240	-	-	-	-	-	-	-	0.450	-	-	-	-	Navarro et al. (2017)
Tomato	fruit	Solanum lycopersicum L.	Fruit	Laboratory study, experimental pot	Chemical Specific, Treatment 2, ND - 0.23	-	Cp/Cs	g dw/ g dw	11.55%	69.820	-	5.060	-	-	-	0.020	-	-	-	-	-	-	-	-	-	-	-	-	Navarro et al. (2017)
Tomato	leaf	Solanum lycopersicum L.	Other - vegetative compartment	Laboratory study, experimental pot	Chemical Specific, Treatment 2, ND - 0.23	-	Cp/Cs	g dw/ g dw	11.55%	-	-	-	-	4.140	-	-	-	-	-	-	-	-	-	0.360	-	-	-	-	Navarro et al. (2017)
Tomato	root	Solanum lycopersicum L.	Other - vegetative compartment	Laboratory study, experimental pot	Chemical Specific, Treatment 2, ND - 0.23	-	Cp/Cs	g dw/ g dw	11.55%	-	-	-	-	1.540	-	0.220	-	-	-	-	-	-	-	1.440	-	-	-	-	Navarro et al. (2017)
Tomato	stem	Solanum lycopersicum L.	Other - vegetative compartment	Laboratory study, experimental pot	Chemical Specific, Treatment 2, ND - 0.23	-	Cp/Cs	g dw/ g dw	11.55%	21.880	-	-	-	0.350	-	0.100	-	-	-	-	-	-	-	0.050	-	-	-	-	Navarro et al. (2017)
Maize	ears	Not available	Grains	Laboratory study, experimental pot	1000	-	Cears/Cs	g dw/ g dw	NA	-	-	-	-	0.004	-	-	-	-	-	-	-	-	-	0.003	-	-	-	-	Stahl et al. (2009); Ghisi et al. (2019)
Maize	ears	Not available	Grains	Laboratory study, experimental pot	250	-	Cears/Cs	g dw/ g dw	NA	-	-	-	-	0.008	-	-	-	-	-	-	-	-	-	0.000	-	-	-	-	Stahl et al. (2009); Ghisi et al. (2019)
Maize	straw	Not available	Animal feed	Laboratory study, experimental pot	1000	-	Cstraw/Cs	g dw/ g dw	NA	-	-	-	-	0.126	-	-	-	-	-	-	-	-	-	0.104	-	-	-	-	Stahl et al. (2009); Ghisi et al. (2019)
Maize	straw	Not available	Animal feed	Laboratory study, experimental pot	250	-	Cstraw/Cs	g dw/ g dw	NA	-	-	-	-	0.272	-	-	-	-	-	-	-	-	-	0.132	-	-	-	-	Stahl et al. (2009); Ghisi et al. (2019)
Oat	straw	Not available	Animal feed	Laboratory study, experimental pot	1000	-	Cstraw/Cs	g dw/ g dw	NA	-	-	-	-	0.690	-	-	-	-	-	-	-	-	-	0.150	-	-	-	-	Stahl et al. (2009); Ghisi et al. (2019)
Oat	grain	Not available	Grains	Laboratory study, experimental pot	1000	-	Cgrain/Cs	g dw/ g dw	NA	-	-	-	-	0.054	-	-	-	-	-	-	-	-	-	0.017	-	-	-	-	Stahl et al. (2009); Ghisi et al. (2019)
Oat	grain	Not available	Grains	Laboratory study, experimental pot	250	-	Cgrain/Cs	g dw/ g dw	NA	-	-	-	-	0.048	-	-	-	-	-	-	-	-	-	0.004	-	-	-	-	Stahl et al. (2009); Ghisi et al. (2019)
Oat	straw	Not available	Animal feed	Laboratory study, experimental pot	250	-	Cstraw/Cs	g dw/ g dw	NA	-	-	-	-	0.880	-	-	-	-	-	-	-	-	-	0.224	-	-	-	-	Stahl et al. (2009); Ghisi et al. (2019)
Spring Wheat grains		Not available	Grains	Laboratory study, experimental pot	1000	-	Cgrain/Cs	g dw/ g dw	NA	-	-	-	-	0.009	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Stahl et al. (2009); Ghisi et al. (2019)
Spring Wheat grains		Not available	Grains	Laboratory study, experimental pot	250	-	Cgrain/Cs	g dw/ g dw	NA	-	-	-	-	0.096	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Stahl et al. (2009); Ghisi et al. (2019)
Spring Wheat straw		Not available	Animal feed	Laboratory study, experimental pot	1000	-	Cstraw/Cs	g dw/ g dw	NA	-	-	-	-	1.900	-	-	-	-	-	-	-	-	-	0.270	-	-	-	-	Stahl et al. (2009); Ghisi et al. (2019)
Spring Wheat straw		Not available	Animal feed	Laboratory study, experimental pot	250	-	Cstraw/Cs	g dw/ g dw	NA	-	-	-	-	3.200	-	-	-	-	-	-	-	-	-	0.200	-	-	-	-	Stahl et al. (2009); Ghisi et al. (2019)
Wheat	grain	Triticum aestivum L.	Grains	Field study	Chemical specific, Plot 1, ND - 10.4	-	Cgrain/Cs	g dw/ g dw	1.42%	0.916	-	0.291	-	0.233	0.254	-	-	-	-	-	-	0.188	-	0.077	-	-	-	-	Wen et al. (2014)
Wheat	grain	Triticum aestivum L.	Grains	Field study	Chemical specific, Plot 2, ND - 25.8	-	Cgrain/Cs	g dw/ g dw	2.29	1.000	-	0.391	-	0.160	0.324	-	-	-	-	-	-	0.133	-	0.062	-	-	-	-	Wen et al. (2014)
Wheat	grain	Triticum aestivum L.	Grains	Field study	Chemical specific, Plot 3, 0.39-28.3	-	Cgrain/Cs	g dw/ g dw	2.53	0.743	-	0.272	0.220	0.133	0.178	0.113	-	-	-	-	-	0.126	-	0.061	-	-	-	-	Wen et al. (2014)
Wheat	grain	Triticum aestivum L.	Grains	Field study	Chemical specific, Plot 4, 0.89-40.8	-	Cgrain/Cs	g dw/ g dw	2.76	0.481	0.531	0.330	0.258	0.111	0.139	0.121	-	-	-	-	-	0.125	-	0.062	-	-	-	-	Wen et al. (2014)
Wheat	root	Triticum aestivum L.	Other - vegetative compartment	Field study	Chemical specific, Plot 1, ND - 10.4	-	Croot/Cs	g dw/ g dw	1.42%	4.440	-	4.570	4.790	4.940	4.150	-	5.180	-	-	3.750	-	2.750	-	1.620	-	-	-	-	Wen et al. (2014)
Wheat	root	Triticum aestivum L.	Other - vegetative compartment	Field study	Chemical specific, Plot 2, ND - 25.8	-	Croot/Cs	g dw/ g dw	2.29	4.090	4.220	3.100	3.550	2.510	2.710	2.640	4.050	-	-	2.860	-	2.100	-	1.190	-	-	-	-	Wen et al. (2014)
Wheat	root	Triticum aestivum L.	Other - vegetative compartment	Field study	Chemical specific, Plot 3, 0.39-28.3	-	Croot/Cs	g dw/ g dw	2.53	2.470	3.440	2.640	2.410	1.940	2.850	2.140	3.350	-	-	2.820	1.650	2.110	-	1.330	-	-	-	-	Wen et al. (2014)
Wheat	root	Triticum aestivum L.	Other - vegetative compartment	Field study	Chemical specific, Plot 4, 0.89-40.8	-	Croot/Cs	g dw/ g dw	2.76	2.700	3.600	2.830	2.680	1.730	2.860	1.990	3.210	-	-	2.070	1.910	1.940	-	1.360	-	-	-	-	Wen et al. (2014)
Wheat	straw	Triticum aestivum L.	Animal feed	Field study	Chemical specific, Plot 1, ND - 10.4	-	Cstraw/Cs	g dw/ g dw	1.42%	2.560	-	1.210	1.610	1.540	1.220	-	-	-	-	-	-	0.666	-	0.332	-	-	-	-	Wen et al. (2014)

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Plant	Plant Compartment Analyzed	Plant Species	Plant Category	Type of Study Design	Soil Concentration (ng/g)	Solution Concentration (ng/L)	Equation	Unit	% OC	Transfer Factors														Reference							
										PFBA	PFPeA	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFUnA	PFDaA	PFTeDA	PFBS	PFHxS	PFHpS	PFOS		PFOSA	PFDS	PFOS from degradation of PFOSA				
Wheat	straw	Triticum aestivum L.	Animal feed	Field study	Chemical specific, Plot 2, ND - 25.8	-	Cstraw/Cs	g dw/ g dw	2.29	2.490	1.890	1.250	1.630	0.764	1.160	0.643	1.150	-	-	0.811	-	0.465	-	0.238	-	-	-	Wen et al. (2014)			
Wheat	straw	Triticum aestivum L.	Animal feed	Field study	Chemical specific, Plot 3, 0.39-28.3	-	Cstraw/Cs	g dw/ g dw	2.53	2.060	1.780	1.110	0.989	0.747	0.649	0.671	0.677	-	-	0.872	-	0.441	-	0.256	-	-	-	Wen et al. (2014)			
Wheat	straw	Triticum aestivum L.	Animal feed	Field study	Chemical specific, Plot 4, 0.89-40.8	-	Cstraw/Cs	g dw/ g dw	2.76	1.640	1.630	1.350	1.230	0.847	0.973	0.803	0.899	-	-	0.503	0.635	0.427	-	0.270	-	-	-	Wen et al. (2014)			
Wheat Husk	husk	Triticum aestivum L.	Animal feed	Field study	Chemical specific, Plot 4, 0.89-40.8	-	Chusk/Cs	g dw/ g dw	2.76%	0.430	-	-	-	0.160	-	-	-	-	-	-	-	-	-	0.054	-	-	-	Wen et al. (2014); Ghisi et al. (2019)			
Alfalfa	root	Medicago sativa L. cv. Chaoren	Other - vegetative compartment	Laboratory study, experimental pot	PFOA = 416.8, PFOS = 154.4	-	croot/Cs	g dw/ g dw	1.93%	-	-	-	-	10.300	-	-	-	-	-	-	-	-	-	-	-	-	3.120	-	-	-	Wen et al. (2016)
Alfalfa	shoot	Medicago sativa L. cv. Chaoren	Animal feed/other vegetables	Laboratory study, experimental pot	PFOA = 416.8, PFOS = 154.4	-	Cshoot/Cs	g dw/ g dw	1.93%	-	-	-	-	3.150	-	-	-	-	-	-	-	-	-	-	-	-	0.407	-	-	-	Wen et al. (2016)
Lettuce	root	Lactuca sativa L.	Other - vegetative compartment	Laboratory study, experimental pot	PFOA = 416.8, PFOS = 154.4	-	croot/Cs	g dw/ g dw	1.93%	-	-	-	-	6.050	-	-	-	-	-	-	-	-	-	-	-	-	3.890	-	-	-	Wen et al. (2016)
Lettuce	shoot	Lactuca sativa L.	Leafy green	Laboratory study, experimental pot	PFOA = 416.8, PFOS = 154.4	-	Cshoot/Cs	g dw/ g dw	1.93%	-	-	-	-	1.180	-	-	-	-	-	-	-	-	-	-	-	-	0.396	-	-	-	Wen et al. (2016)
Maize	root	Zea mays L. cv. Nongda 108	Other - vegetative compartment	Laboratory study, experimental pot	PFOA = 416.8, PFOS = 154.4	-	croot/Cs	g dw/ g dw	1.93%	-	-	-	-	1.690	-	-	-	-	-	-	-	-	-	-	-	-	2.650	-	-	-	Wen et al. (2016)
Maize	shoot	Zea mays L. cv. Nongda 108	Animal feed	Laboratory study, experimental pot	PFOA = 416.8, PFOS = 154.4	-	Cshoot/Cs	g dw/ g dw	1.93%	-	-	-	-	0.206	-	-	-	-	-	-	-	-	-	-	-	-	0.165	-	-	-	Wen et al. (2016)
Mung bean	root	Vigna radiata L. Wilczek	Other - vegetative compartment	Laboratory study, experimental pot	PFOA = 416.8, PFOS = 154.4	-	croot/Cs	g dw/ g dw	1.93%	-	-	-	-	7.750	-	-	-	-	-	-	-	-	-	-	-	-	4.140	-	-	-	Wen et al. (2016)
Mung bean	shoot	Vigna radiata L. Wilczek	legume	Laboratory study, experimental pot	PFOA = 416.8, PFOS = 154.4	-	Cshoot/Cs	g dw/ g dw	1.93%	-	-	-	-	8.400	-	-	-	-	-	-	-	-	-	-	-	-	0.683	-	-	-	Wen et al. (2016)
Radish	root	Raphanus sativus L. cv. Dahongpao	Root vegetable (edible)	Laboratory study, experimental pot	PFOA = 416.8, PFOS = 154.4	-	Croot/Cs	g dw/ g dw	1.93%	-	-	-	-	3.000	-	-	-	-	-	-	-	-	-	-	-	-	2.610	-	-	-	Wen et al. (2016)
Radish	shoot	Raphanus sativus L. cv. Dahongpao	Other - vegetative compartment	Laboratory study, experimental pot	PFOA = 416.8, PFOS = 154.4	-	Cshoot/Cs	g dw/ g dw	1.93%	-	-	-	-	5.340	-	-	-	-	-	-	-	-	-	-	-	-	0.468	-	-	-	Wen et al. (2016)
Ryegrass	root	Lolium multiflorum Lam.	Other - vegetative compartment	Laboratory study, experimental pot	PFOA = 416.8, PFOS = 154.4	-	Croot/Cs	g dw/ g dw	1.93%	-	-	-	-	2.350	-	-	-	-	-	-	-	-	-	-	-	-	1.370	-	-	-	Wen et al. (2016)
Ryegrass	shoot	Lolium multiflorum Lam.	Animal feed	Laboratory study, experimental pot	PFOA = 416.8, PFOS = 154.4	-	Cshoot/Cs	g dw/ g dw	1.93%	-	-	-	-	1.320	-	-	-	-	-	-	-	-	-	-	-	-	0.181	-	-	-	Wen et al. (2016)
Soy bean	root	Glycine max L. Merrill	Other - vegetative compartment	Laboratory study, experimental pot	PFOA = 416.8, PFOS = 154.4	-	Croot/Cs	g dw/ g dw	1.93%	-	-	-	-	3.210	-	-	-	-	-	-	-	-	-	-	-	-	4.680	-	-	-	Wen et al. (2016)
Soy bean	shoot	Glycine max L. Merrill	legume	Laboratory study, experimental pot	PFOA = 416.8, PFOS = 154.4	-	Cshoot/Cs	g dw/ g dw	1.93%	-	-	-	-	0.296	-	-	-	-	-	-	-	-	-	-	-	-	0.258	-	-	-	Wen et al. (2016)
Grass	grass	Not available	Animal feed	Not available	Not available	-	Cgrass/Cs	g dw/ g dw	NA	-	-	3.400	0.900	0.250	0.120	0.100	-	-	-	-	-	-	-	-	-	-	0.070	-	-	-	Yoo et al. (2011) as cited in Blaine et al. (2013)
Rapeseed	whole plant	Brassica campestris L.	Other vegetables	Laboratory study, experimental pot	PFOA = 285, PFOS=264	-	Cplant/Cs	g dw/ g dw	1.81%	-	-	-	-	0.058	-	-	-	-	-	-	-	-	-	-	-	-	0.025	-	-	-	Zhao et al. (2017)
Rapeseed	root	Brassica campestris L.	Other - vegetative compartment	Laboratory study, experimental pot	PFOA = 285, PFOS=264	-	Croot/Cs	g dw/ g dw	1.81%	-	-	-	-	0.090	-	-	-	-	-	-	-	-	-	-	-	-	0.091	-	-	-	Zhao et al. (2017)
Rapeseed	shoot	Brassica campestris L.	Animal feed	Laboratory study, experimental pot	PFOA = 285, PFOS=264	-	Cshoot/Cs	g dw/ g dw	1.81%	-	-	-	-	0.052	-	-	-	-	-	-	-	-	-	-	-	-	0.011	-	-	-	Zhao et al. (2017)
Wheat	plant	Triticum aestivum L.	Grains	Laboratory study, experimental pot	PFOA = 285, PFOS=264	-	Cp/Cs	g dw/ g dw	1.81%	-	-	-	-	0.012	-	-	-	-	-	-	-	-	-	-	-	-	0.016	-	-	-	Zhao et al. (2017)
Wheat	root	Triticum aestivum L.	Other - vegetative compartment	Laboratory study, experimental pot	PFOA = 285, PFOS=264	-	Croot/Cs	g dw/ g dw	1.81%	-	-	-	-	0.030	-	-	-	-	-	-	-	-	-	-	-	-	0.073	-	-	-	Zhao et al. (2017)
Wheat	shoot	Triticum aestivum L.	Animal feed	Laboratory study, experimental pot	PFOA = 285, PFOS=264	-	Cshoot/Cs	g dw/ g dw	1.81%	-	-	-	-	0.008	-	-	-	-	-	-	-	-	-	-	-	-	0.005	-	-	-	Zhao et al. (2017)
Pumpkin	root	Cucurbita maxima L.	Other - vegetative compartment	Laboratory study, experimental pot	-	926	Cr/Cw	ml/ g dw	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	19.300	-	-	-	Zhao et al. (2018)
Soybean	root	Glycine max L. Merrill	Other - vegetative compartment	Laboratory study, experimental pot	-	926	Cr/Cw	ml/ g dw	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	19.400	-	-	-	Zhao et al. (2018)

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Plant	Plant Compartment Analyzed	Plant Species	Plant Category	Type of Study Design	Soil Concentration (ng/g)	Solution Concentration (ng/L)	Equation	Unit	% OC	Transfer Factors															Reference				
										PFBA	PFPeA	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFUnA	PFDoA	PFTTrDA	PFTeDA	PFBS	PFHxS	PFHpS	PFOS		PFOSA	PFDS	PFOS from degradation of PFOSA	
Pumpkin	shoot	Cucurbita maxima L.	Other vegetables	Laboratory study, experimental pot	-	926	Cshoot/Cw	ml/ g dw	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.737	-	-	Zhao et al. (2018), calculated by Arcadis	
Soybean	shoot	Glycine max L. Merrill legume		Laboratory study, experimental pot	-	926	Cshoot/Cw	ml/ g dw	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.164	-	-	Zhao et al. (2018), calculated by Arcadis	
Wheat	above ground compartment	Triticum aestivum L.	Grains	Laboratory study, experimental pot, salinity 0%	-	1000	Cp/Cw	ml/ g ww	-	0.850	-	-	0.460	0.430	-	-	-	0.330	-	-	-	-	-	-	-	-	-	-	Zhao et al. 2016
Wheat	above ground compartment	Triticum aestivum L.	Grains	Laboratory study, experimental pot, salinity 0.1%	-	1000	Cp/Cw	ml/ g ww	-	1.060	-	-	0.820	0.760	-	-	-	0.670	-	-	-	-	-	-	-	-	-	-	Zhao et al. 2016
Wheat	above ground compartment	Triticum aestivum L.	Grains	Laboratory study, experimental pot, salinity 0.2%	-	1000	Cp/Cw	ml/ g ww	-	1.340	-	-	1.120	1.010	-	-	-	0.770	-	-	-	-	-	-	-	-	-	-	Zhao et al. 2016
Wheat	above ground compartment	Triticum aestivum L.	Grains	Laboratory study, experimental pot salinity 0.3%	-	1000	Cp/Cw	ml/ g ww	-	2.000	-	-	1.390	1.490	-	-	-	0.940	-	-	-	-	-	-	-	-	-	-	Zhao et al. 2016
Wheat	above ground compartment	Triticum aestivum L.	Grains	Laboratory study, experimental pot salinity 0.4%	-	1000	Cp/Cw	ml/ g ww	-	2.610	-	-	2.100	2.090	-	-	-	1.590	-	-	-	-	-	-	-	-	-	-	Zhao et al. 2016

Notes
Cears = ears concentration
Cfruit = fruit concentration
Cgrain = grain concentration
Chead = head concentration
Chusk = husk concentration
Cleaf = leaf concentration
Cp = plant concentration
Cpeels = peels concentration
Croot = root concentration
Cs = soil concentration
Cshoot = shoot concentration
Cstraw = straw concentration
Ctwig = twig concentration
Cw = water solution concentration
Ctuber = tuber concentration

- not available
g = grams
g dm soil = grams root tissue mass
g dw = grams, dry weight
g ww = grams, wet weight
L = liters
ml = milliliters
ng = nanograms
ug = micrograms

This section updates the findings of several studies that reviewed and compiled soil-to-plant uptake factors for PFAS (e.g., Intrinsik 2018 for PFOA and PFOS, and Ghisi et al. 2019 for PFBA, PFOA, PFBS, and PFOS). Soil- or solution-to-plant uptake factors are referred to as transfer factors (TFs) in this review. TF is used as a generic term to encompass both bioaccumulation and bioconcentration factors that are usually used in the literature to define the ratio of the concentration of a chemical in plant tissue to the concentration in soil or solution. This update includes data from recent studies as well as TFs for several homologues of PFAS including PFCAs (C4-C14), PFSAAs (C4-C10), and PFOSA. TFs from soil or solution to plants are available for diversity of plant species and tissue types and are summarized in Table B-1 (Appendix B).

Based on review of available information on plant uptake of PFOS and PFOA, Intrinsik (2018) concluded that, in general, plant tissues with high water content (e.g., vegetables) exhibit higher bioaccumulation than cereal crops (e.g., wheat, ryegrass, corn). Based on a review of bioaccumulation of PFAS in agricultural plants, Ghisi et al. (2019) concluded that the available data suggest a direct correlation between PFAS concentrations in soil and bioaccumulation in plants. Ghisi et al. (2019) also found that PFAS chain length, functional groups, plant species, and plant tissue type substantially influence plant uptake of PFAS.

Stahl et al. (2009) studied the soil-to-plant uptake of PFAS in spring wheat, oats, potatoes, maize, and ryegrass at five different soil concentrations (i.e., 0.25, 1, 10, 10, 25, 50 milligrams per kilogram [mg/kg]). No changes in the yield of cultivated crops treated with PFAS at various soil concentrations were noted compared with the controls. Ghisi et al. (2019) used the data on PFOA and PFOS concentrations in plant tissue and calculated the TFs for various parts of analyzed crops at soil concentration of 0.25 and 1 mg/kg. Table B-1 presents the TFs for soil to maize straw, maize ears, oat grain, oat straw, wheat grains, wheat straw, and ryegrass (four cuttings) for PFOA and PFOS.

Lechner and Knapp (2011) studied the distribution of PFOA and PFOS in greenhouse-grown carrots, potatoes, and cucumbers to understand the difference in the distribution of PFOA and PFOS between below- and aboveground plant tissues. Sewage sludge containing PFOA and PFAS was mixed with soil at rates consistent with German regulations for the application of sludge to agricultural lands. The concentrations of PFOA and PFOS in vegetative parts of all plants were 10 times higher than the concentrations in the edible parts of vegetation. More than 80 percent of the PFOA and PFOS mass taken up by all three vegetables was stored in vegetated (non-edible) parts of plants. This observation was only seen for accumulation of PFOA and PFOS in carrots and potatoes; short-chain PFAS are likely to demonstrate a different distribution pattern among various parts of carrots and potatoes.

Blaine et al. (2013) investigated the bioaccumulation of several PFAA in edible parts of greenhouse-grown lettuce and tomato. Three types of soils were included: industrially impacted biosolid-amended soil, municipal biosolids-amended soil, and a control soil. Short-chain PFAA (i.e., PFBA in lettuce and PFPeA in tomato) showed the highest bioaccumulation in tested plants. TF decreased with increasing carbon chain length. Blaine et al. (2013) concluded that the bioaccumulation of PFAAs from soil depends on PFAA concentration, the specific PFAA, soil properties, and type of crop.

In another greenhouse study, Blaine et al. (2014a) investigated the uptake of PFAA by radish, celery, tomato, and sugar snap pea using the same soil treatments as in Blaine et al. (2013). TFs were calculated for root tissue, shoot tissue, and fruit tissue. No chain length dependency was observed for the RCFs for tomato and pea, while the RCFs for radish and celery showed a slight decrease with increasing chain length. Chain length dependency (i.e., decrease in uptake with increasing chain length) for shoot-

to-soil concentration factors (SCFs) was noted for all crops. In general, the concentrations of long-chain PFAA were lower than the concentrations of short-chain PFAA in fruit crops.

Blaine et al. (2014b) investigated the effect of impacted irrigation water on the uptake of PFAS in lettuce and strawberry including using varying organic carbon content (i.e., 0.4, 2, and 6 percent) in the experiments with lettuce. Bioaccumulation of PFAS in lettuce was lowest in soil with 6 percent organic carbon content and was affected by chain length and functional groups. The TFs presented in this study are based on soil concentrations estimated using K_d values rather than empirical soil analysis introducing uncertainty to the reported TFs.

Wen et al. (2014) investigated the uptake of PFCA and PFSA by various parts of wheat grown in biosolid-amended agricultural fields. PFAS concentrations were measured in soil, roots, straw, husk, and grain tissue under four different soil characteristics where the annual biosolid application rate ranged from 4.5 tons per hectare per year (t/ha/y) to 36 t/ha/y. Roots exhibited the greatest accumulation of PFAA followed by straw, grain, and husks. The relationship between the concentration of PFSA in soil and wheat grains was linear; for PFCA, the relationship was logarithmic. The difference in relationship between soil and grain concentrations for PFCA and PFSA suggests different uptake mechanisms for these two groups of PFAA. PFCA had higher root-to-straw TFs than PFSA. Furthermore, short-chain PFCA had higher root-to-straw TFs than long-chain PFCA. The chain length dependence is consistent with previous studies and suggests that the transport of chemicals from root to shoot is mainly through transpiration. Both direct xylem transport from root to grain and relocation from straw to grain were transport mechanisms contributing to bioaccumulation of PFAS in wheat grains. Soil-to-root, straw, and grain TFs are summarized in Table B-1.

Felizeter et al. (2014) investigated the accumulation of PFAA in various compartments of hydroponically greenhouse-grown tomato, cabbage, and zucchini plants including roots, stems, leaves, twigs, and edible parts. PFAA with carbon chain length of greater than 11 were accumulated in the roots of all three plant species but were not detected in the edible parts. All other PFAA homologues were detected in other aboveground plant tissues with the transpiration stream concentration factor ranging from 0.05 to 0.25 depending on PFAA homologue. This study concluded that, in general, the uptake of PFAA from solution and their distribution to various parts of plants is similar among tomato, zucchini, and cabbage. Because TFs were presented in figures rather than tables. The TFs shown in Table B-1 were calculated based on raw data presented in Tables S11 to S13 for cabbage, zucchini, and tomato (Felizeter et al. 2014).

Krippner et al. (2015) investigated the uptake of PFCA and PFSA by maize kernels and maize straw from soil at two soil concentrations of 0.25 and 1 mg/kg during a laboratory study. Consistent with other studies, the concentration of PFCA in straw of maize decreases with increasing carbon chain length. The authors analyzed the effect of initial soil concentration in bioaccumulation of PFAS in maize straw and grains. The analytical results showed that a four-fold increase in soil concentration reduces the soil to straw TFs for short-chain PFAS (PFBA, PFPeA, PFBS). In contrast, increasing soil concentration increases the TFs for long-chain PFAS, with the greatest increase occurring for PFOS (doubled the TFs at higher soil concentration). The soil-to-grain TFs were almost doubled for PFBA, PFHxA, and PFHpA (~1.7). Long-chain PFAS were not detected in maize grain, precluding calculation of TFs for that tissue (Krippner et al. 2015). The soil-to-straw and soil-to-grain TFs calculated for soil concentrations of 0.25 mg/kg and 1 mg/kg are summarized in Table B-1.

Wen et al. (2016) investigated the role of protein and lipid content of plant tissue on the accumulation of PFOS and PFOA in roots and shoots of several plants including alfalfa, lettuce, maize, mung bean, radish, ryegrass, and soybean. The protein content in roots ranged from 3.35 percent in ryegrass to 10.4

percent in mung bean and in shoots from 6.37 percent in maize to 29.1 percent in mung bean. A positive correlation was observed between accumulation of PFOA and PFOS and the protein content in roots and shoots, while a negative correlation was observed between PFOA and PFOS accumulation and the lipid content of roots. The inhibition of accumulation with increasing lipid content was greater for PFOA than PFOS. The results showed that legume crops with high protein content (i.e., mung beans) exhibit higher soil-to-plant TFs than other vegetable crops (e.g., lettuce). This observation was assumed to be associated with the protein content of plant tissues, given that PFAS tend to bind to protein rather than lipids. The soil-to-root and soil-to-shoot TFs reported by Wen et al. (2016) are shown in Table B-1.

Zhao et al. (2016) investigated the effect of salinity and temperature on uptake by wheat of PFCA in solution in a hydroponic culture system. The concentration of PFCA in the solution was kept at 1 microgram per milliliter ($\mu\text{g/ml}$). A linear increasing relationship between plant uptake of PFCA and salinity and temperature was reported, where an increase in salinity and temperature led to both an increase in root uptake from solution and also an increase in translocation of PFCA from roots to shoots. Except for PFBA, the amount of PFCA in roots was higher than in shoots. The TFs reported at 0, 0.1, 0.2, 0.3, and 0.4 percent salinity are presented in Table B-1.

Bizkarguenaga et al. (2016) studied the uptake of PFOA, PFOS, and PFOSA in various parts of carrots and lettuce grown in two types of compost-amended soil: 1) substrate (OC = 53 percent) and 2) soil (OC = 2.3 percent) in a greenhouse experimental study. PFAS were analyzed in the peel, core, and leaves of carrots and in the heart and leaves of lettuce. PFOA and PFOS accumulated more in carrot leaves than in carrot peel or core. PFOSA was not detected in soil or carrot after carrot cultivation, while a high concentration of PFOS was measured in both soil and carrot, which may be due to degradation of PFOSA. Twice as much PFOA accumulated in lettuce hearts than leaves. Accumulation of PFOS in lettuce hearts was more than one order of magnitude greater than accumulation in leaves. Overall, however, PFOA accumulates more than PFOS in lettuce, likely due to its higher water solubility (Bizkarguenaga et al. 2016). Total organic carbon was identified as the key soil parameter influencing PFOA and PFOS uptake in carrots with TFs decreasing with increasing soil organic carbon content. For lettuce, the organic carbon content of soil appears to affect the degradation of PFOSA to PFOS with a higher degradation rate observed at higher soil organic carbon content. No influence of soil type in accumulation of PFOSA was observed in lettuce. However, in the case of PFOS degraded from PFOSA, higher accumulation at lower soil organic carbon content was observed, similar to carrot. No degradation of PFOSA was observed in soil in absence of any crops.

Navarro et al. (2017) investigated the bioaccumulation of PFAS in spinach and tomatoes grown in pots with biosolid-amended soil and corn grown in spiked soil during a laboratory study. Two different organic wastes were applied once to soil at an agronomic rate suitable for nitrogen to represent the use of biosolids as fertilizer for agricultural lands. The corn was grown in a spiked soil at a high PFOS concentration of 50 mg/kg to represent a worse-case scenario. The distribution of PFAS in root, stem, leaf, and fruits was investigated. Navarro et al. (2017) found that long-chain PFAS accumulate in roots, while shorter-chain PFAS accumulate in aboveground plant tissues. TFs among various plant tissues were also calculated, and the findings suggest that the type of crop substantially influences accumulation various plant tissues. The calculated TFs for spinach, tomato (root, stem, leaf and fruit), and corn (root and leaf) from this study were summarized in Table B-1.

Zhao et al. (2017) studied the interaction of PFOA and PFOS as well as cadmium on soil enzyme activity, phytotoxicity, and their bioaccumulation in wheat and rapeseed. Soil samples were collected from a farm in China and spiked with cadmium and then PFOS and PFOA at concentrations found in the environment (e.g., the group I treatment soils had PFOA concentrations of 0.285 $\mu\text{g/g}$ and 0.264 $\mu\text{g/g}$). The results

suggest that accumulation and translocation of PFOA and PFOS from root to shoots in wheat were diminished in the presence of cadmium in soil. However, for rapeseed, while the accumulation of PFOA and PFOS was decreased, the translocation of PFOA and PFOS from roots to shoots was improved in the presence of cadmium. This study concluded that the bioavailability of PFAS in soil for plant uptake is reduced in presence of cadmium. The TFs developed in this study in absence of cadmium are presented in Table B-1.

Zhao et al. (2018) investigated the biotransformation and enzymatic responses in pumpkin and soybean as a result of exposure to PFOSA in solutions. PFOSA was degraded to PFSA's including PFOS, PFHxS, and PFBS in both pumpkin and soybean, and the concentrations of PFOSA and the degradation products were measured in both roots and shoots. PFOSA and PFOS exhibited the greatest accumulation in roots, followed by PFHxS and PFBS. The results indicated activation of antioxidant system in plants as a result of exposure to PFOSA and its degradation products. The reported root TFs for PFOSA are presented in Table B-1.

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A decorative graphic consisting of three thin orange lines. One line is horizontal, extending across the width of the page. Two other lines are diagonal, starting from the bottom left and extending towards the top right, crossing the horizontal line.